Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
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Thermal fluctuations and conformational effects on NMR parameters in b-O-4 lignin dimer from QM/MM and machine-learning approaches.

aSonia Milena Aguilera-Segura, bDominik Dragún, aRobin Gaumard, aFrancesco Di Renzo, cIrina Malkin Ondík ,aTzonka Mineva*

a.ICGM, Univ Montpellier, CNRS, ENSCM, Montpellier, France
b.FIIT STU in Bratislava, Ilkovičova 2, 842 16 Bratislava, Slovakia
c.MicroStep-MIS spol. s.r.o. Čavojského 1, 84104 Bratislava, Slovakia

* To whom correspondence should be addressed
Email: tzonka.mineva@enscm.fr

SUPPORTING FILE 6

Number of atoms, Chemical element, Cartesian coordinates in Å, and isotropic shielding in ppm in G-b-G in acetonitrile-water solvent.

55
name= lig-ACN-Water-frame_1

C	-4.231705	-0.157120	-3.013888	55.04
H	-4.362730	-1.194885	-3.312966	31.24
C	-3.741873	1.306243	-1.079067	77.38
H	-3.552850	1.283028	-0.032373	26.56
C	-3.821281	2.446927	-1.850152	9.43
O	-3.577439	3.768186	-1.443690	201.80
C	-3.805614	4.158266	-0.068181	105.87
H	-3.533470	3.277493	0.597955	26.62
H	-4.900147	4.461475	-0.026980	24.91
H	-3.115440	4.996081	0.057729	26.93
C	-4.166443	2.272679	-3.245507	5.06
O	-4.366232	3.358295	-4.209514	91.80
H	-4.312530	4.329231	-3.779091	22.38
C	-4.269978	1.035914	-3.834904	71.42
H	-4.542809	0.912285	-4.842170	15.83
C	-3.968790	0.034402	-1.649180	-4.09
C	-4.076105	-1.231766	-0.801259	77.82
H	-4.795974	-1.938315	-1.244526	24.35
O	-4.761559	-1.016034	0.497132	106.87
H	-4.152488	-0.604670	1.275471	21.60
C	-2.727890	-1.964461	-0.653841	96.27
H	-2.213442	-2.345765	-1.624625	26.40
C	-2.852421	-3.260635	0.200522	117.73
O	-3.490869	-4.374180	-0.484670	177.67
H	-2.879950	-4.589270	-1.209197	31.20
H	-3.305047	-3.150655	1.210437	25.94
H	-1.812386	-3.428677	0.380691	27.14
C	1.535822	-1.729685	-0.900455	53.29
H	1.985900	-2.095028	-1.805662	19.37
C	1.585884	-0.311724	1.081426	48.49
H	2.263632	0.309765	1.714437	22.49
C	0.160279	-0.366410	1.156342	8.49
O	-0.664166	0.182953	2.141195	191.66
C	0.016042	0.488027	3.407188	115.81
H	-0.763449	0.529445	4.155870	26.65
H	0.834398	-0.217420	3.554529	26.39
H	0.364401	1.523833	3.325008	25.67
C	-0.535806	-1.182954	0.183415	9.10

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 O      -1.932266    -1.075649     0.173969     143.74
 C       0.143142    -1.787029    -0.891126      70.89
 H      -0.285203    -2.348944    -1.701507      23.53
 C       2.238040    -0.967167     0.007679      31.14
 C       3.767158    -0.805436    -0.191207      72.78
 H       4.079777    -1.049448    -1.275265      20.88
 O       4.139601     0.536339     0.206537     285.02
 H       5.091848     0.615618     0.125681      19.11
 C       4.643008    -1.855777     0.628942      81.33
 H       4.581520    -1.792944     1.783594      23.93
 O       4.242189    -3.206389     0.220211     363.88
 H       4.461989    -3.294095    -0.739609      29.69
 C       6.155408    -1.663210     0.203988      97.65
 O       6.529064    -0.260663     0.122389     326.94
 H       6.984360    -0.137924     0.944780      30.69
 H       6.280170    -2.119625    -0.831330      31.85
 H       6.873864    -2.199779     0.875990      29.27
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name= lig-ACN-Water-frame_2
 C      -4.177511    -0.124849    -3.016325      62.11
 H      -4.225444    -1.070403    -3.602139      23.00
 C      -3.721045     1.281383    -1.084406      53.39
 H      -3.389663     1.504001    -0.054374      22.15
 C      -3.865007     2.465018    -1.927900      -2.25
 O      -3.583338     3.737576    -1.478400     205.93
 C      -3.798908     4.111620    -0.073509     105.85
 H      -3.605669     3.334417     0.755010      25.29
 H      -4.864865     4.471449     0.153571      24.41
 H      -3.147650     5.033922     0.200442      25.26
 C      -4.157943     2.358725    -3.314269       7.25
 O      -4.361839     3.328529    -4.173462      88.14
 H      -4.088366     4.310997    -3.869588      20.71
 C      -4.306101     0.987168    -3.828607      30.95
 H      -4.579807     0.894996    -4.848605      23.82
 C      -3.983377    -0.004201    -1.625775      24.72
 C      -4.075683    -1.225910    -0.735363     100.45
 H      -4.692205    -1.955297    -1.321586      27.50
 O      -4.711422    -0.980809     0.491615     201.96
 H      -4.141744    -0.526120     1.164318      24.20
 C      -2.757126    -1.978235    -0.582537      95.10
 H      -2.413639    -1.964062    -1.687038      28.55
 C      -2.799757    -3.279380     0.212875     123.90
 O      -3.484065    -4.370624    -0.491337     160.10
 H      -2.929187    -4.528892    -1.333382      29.91
 H      -3.409191    -3.022307     1.092977      27.23
 H      -1.852694    -3.715498     0.488893      27.27
 C       1.567569    -1.738723    -0.948116      41.76
 H       2.118779    -2.264580    -1.753576      20.25
 C       1.557431    -0.277035     1.032780      35.20
 H       2.003555     0.488158     1.646126      26.67
 C       0.143093    -0.410188     1.122705       4.66
 O      -0.651153     0.164283     2.143846     186.43
 C       0.007145     0.552944     3.386549     119.77
 H      -0.813815     0.486739     4.122449      26.54
 H       0.675455    -0.197821     3.767255      25.63
 H       0.539558     1.527607     3.382830      24.92
 C      -0.565157    -1.141350     0.126764      10.04
 O      -1.919494    -1.083569     0.209548     157.35
 C       0.151688    -1.830652    -0.864168      75.06
 H      -0.465010    -2.456965    -1.531515      26.70
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 C       2.309916    -0.983203     0.016414      -8.21
 C       3.794537    -0.818714    -0.149141     121.82
 H       3.986223    -0.890146    -1.286162      20.65
 O       4.090393     0.588362     0.232957     256.75
 H       5.091470     0.543321     0.055466      16.24
 C       4.666680    -1.874015     0.575134      86.70
 H       4.415030    -1.789499     1.722464      24.58
 O       4.243881    -3.189692     0.253787     366.78
 H       4.208052    -3.263031    -0.751084      27.18
 C       6.131886    -1.696504     0.163579      97.71
 O       6.574400    -0.256875     0.117889     289.59
 H       6.944933     0.077850     0.951782      25.72
 H       6.217222    -2.043103    -0.916663      29.80
 H       6.821149    -2.275906     0.808794      28.37
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name= lig-ACN-Water-frame_3
 C      -4.151169    -0.101532    -3.018888      28.72
 H      -4.360996    -1.145422    -3.402638      18.63
 C      -3.734687     1.320631    -1.156699      68.69
 H      -3.533347     1.378521    -0.041774      22.61
 C      -3.858941     2.425028    -1.936459      12.09
 O      -3.583988     3.755726    -1.480029     219.32
 C      -3.821561     4.084278    -0.051745      95.09
 H      -3.460883     3.197123     0.567810      24.61
 H      -4.932901     4.325433     0.035449      23.47
 H      -3.086822     5.023698     0.048560      23.71
 C      -4.159004     2.270591    -3.333908       7.82
 O      -4.366204     3.389977    -4.207342     176.60
 H      -4.022671     4.197389    -3.777431      21.24
 C      -4.338830     1.027198    -3.861917      68.84
 H      -4.400772     0.952873    -4.947295      27.69
 C      -3.959844     0.006154    -1.613586      14.58
 C      -4.086607    -1.266865    -0.722268      98.05
 H      -4.831448    -1.968973    -1.196747      25.38
 O      -4.730544    -0.938439     0.523353     211.62
 H      -4.169229    -0.582803     1.179146      27.16
 C      -2.713219    -1.955945    -0.530190      95.45
 H      -2.205121    -2.200008    -1.516268      26.88
 C      -2.790974    -3.345749     0.221006     121.46
 O      -3.472306    -4.367534    -0.518853     178.82
 H      -2.854058    -4.761295    -1.218163      28.51
 H      -3.410908    -3.192338     1.098603      27.18
 H      -1.793920    -3.529377     0.669662      26.85
 C       1.592125    -1.752897    -0.938049      43.95
 H       2.162823    -2.402862    -1.652755      19.11
 C       1.516933    -0.253083     0.964300      68.36
 H       2.056175     0.254049     1.710769      25.85
 C       0.162203    -0.436155     1.114796      19.46
 O      -0.609351     0.147603     2.126667     181.13
 C      -0.015800     0.570293     3.403473     125.92
 H      -0.826670     0.915181     4.107733      26.34
 H       0.661007    -0.178333     3.729083      26.69
 H       0.499214     1.542969     3.187404      25.81
 C      -0.553637    -1.100521     0.081062      17.02
 O      -1.934060    -1.067895     0.272444     190.45
 C       0.185645    -1.876634    -0.851612      74.79
 H      -0.280343    -2.491635    -1.667332      24.99
 C       2.257681    -0.972390     0.005181      22.21
 C       3.749112    -0.748513    -0.145873     103.68
 H       4.014691    -0.848979    -1.259035      21.14
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 O       4.088577     0.604960     0.276741     252.42
 H       5.111042     0.711858     0.263784      17.20
 C       4.667780    -1.831726     0.534704      85.79
 H       4.660364    -1.634186     1.704424      23.57
 O       4.230982    -3.216919     0.266971     336.22
 H       4.507692    -3.399303    -0.704723      27.06
 C       6.164241    -1.687152     0.118867     101.43
 O       6.642773    -0.265234     0.118831     316.74
 H       7.157597    -0.225529     0.979289      27.73
 H       6.298219    -2.069274    -0.933255      30.22
 H       6.786918    -2.331406     0.758798      28.98
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name= lig-ACN-Water-frame_4
 C      -4.220870    -0.147132    -3.048856      67.20
 H      -4.351271    -1.176771    -3.465984      30.20
 C      -3.764081     1.287040    -1.097016      49.14
 H      -3.696534     1.459801     0.024141      22.12
 C      -3.821301     2.479705    -1.956133      15.56
 O      -3.599227     3.759865    -1.504798     219.34
 C      -3.820953     4.031621    -0.111128     104.46
 H      -3.427673     3.289062     0.644715      26.56
 H      -4.921272     4.129393     0.175984      25.32
 H      -3.359186     5.106895     0.220630      24.84
 C      -4.177488     2.351552    -3.352365       4.50
 O      -4.345705     3.389566    -4.202347     138.54
 H      -4.370970     4.272718    -3.869549      26.08
 C      -4.291290     0.972947    -3.911348      30.37
 H      -4.556931     0.771654    -4.999481      14.59
 C      -3.944798     0.010486    -1.677674      26.22
 C      -4.072737    -1.232805    -0.732467      58.74
 H      -4.716897    -2.013098    -1.235600      23.76
 O      -4.792598    -0.912411     0.547583     174.67
 H      -4.221488    -0.574714     1.267239      23.66
 C      -2.707842    -2.024537    -0.493642      89.15
 H      -2.251633    -2.148583    -1.490040      25.95
 C      -2.830743    -3.328387     0.300268     121.58
 O      -3.425511    -4.395886    -0.565820     202.32
 H      -2.661437    -4.751918    -1.026796      30.13
 H      -3.348934    -3.232185     1.245045      26.93
 H      -1.814544    -3.772524     0.396502      24.66
 C       1.582530    -1.812466    -0.881930      58.96
 H       2.118299    -2.272305    -1.751588      19.76
 C       1.576470    -0.257749     1.007636      59.30
 H       2.169294     0.267305     1.720470      25.37
 C       0.150121    -0.390918     1.110171      10.59
 O      -0.630856     0.126765     2.138751     188.22
 C       0.014554     0.630486     3.333089     117.76
 H      -0.912143     0.850408     3.941952      25.28
 H       0.502528    -0.104402     3.944776      27.28
 H       0.734053     1.484436     3.190733      25.70
 C      -0.540003    -1.135032     0.103532      15.32
 O      -1.912611    -1.055827     0.306755     144.12
 C       0.178805    -1.863344    -0.892996      77.19
 H      -0.346036    -2.493387    -1.646972      21.42
 C       2.247188    -0.903495    -0.053576      23.16
 C       3.751252    -0.709535    -0.199872      85.11
 H       3.971771    -0.743805    -1.315949      22.23
 O       4.092857     0.624346     0.353064     269.14
 H       5.080814     0.527035     0.357448      17.92
 C       4.687835    -1.785975     0.515976      71.21
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 H       4.567756    -1.744017     1.689086      23.13
 O       4.250849    -3.194264     0.277603     328.88
 H       4.667393    -3.457257    -0.572741      31.08
 C       6.202232    -1.667630     0.045734     111.14
 O       6.708357    -0.328458     0.097544     337.95
 H       7.075296    -0.003718     1.037181      25.78
 H       6.321338    -2.018362    -0.998359      30.72
 H       6.807973    -2.267204     0.728962      28.64
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name= lig-ACN-Water-frame_5
 C      -4.252028    -0.156407    -3.094398      42.41
 H      -4.366365    -1.092838    -3.634889      29.31
 C      -3.816690     1.316800    -1.142105      63.03
 H      -3.676154     1.392206    -0.048097      26.87
 C      -3.821800     2.422237    -1.967408      22.44
 O      -3.611616     3.787190    -1.529499     219.52
 C      -3.857819     4.009904    -0.085703      99.47
 H      -3.155792     3.365189     0.481060      28.05
 H      -4.950093     3.792466     0.097889      26.48
 H      -3.541031     5.159161    -0.038521      24.85
 C      -4.153537     2.279008    -3.354496      18.63
 O      -4.350544     3.375945    -4.241205     139.27
 H      -4.170362     4.246294    -3.772384      23.01
 C      -4.261955     1.012921    -3.880615      52.41
 H      -4.603142     1.007724    -4.991107      16.28
 C      -3.974411    -0.011477    -1.643437      -7.86
 C      -4.069925    -1.210575    -0.690293      82.37
 H      -4.758446    -1.881046    -1.260743      22.96
 O      -4.842247    -0.922485     0.487822     160.94
 H      -4.265320    -0.434196     1.234480      22.80
 C      -2.789990    -1.963759    -0.430952     105.99
 H      -2.414121    -2.203554    -1.408694      28.04
 C      -2.804628    -3.379899     0.289127     118.60
 O      -3.389375    -4.394151    -0.564944     185.56
 H      -2.732173    -4.669421    -1.273809      27.95
 H      -3.447382    -3.286106     1.178580      27.15
 H      -1.780830    -3.542405     0.768139      25.56
 C       1.563229    -1.785018    -0.921221      60.41
 H       2.133683    -2.310323    -1.699953      21.12
 C       1.596902    -0.272471     1.067241      46.60
 H       2.050137     0.480000     1.735017      24.68
 C       0.222700    -0.362284     1.110214      13.53
 O      -0.640535     0.112936     2.129437     185.30
 C       0.003670     0.671263     3.316667     119.98
 H      -0.721026     1.286272     3.923318      26.11
 H       0.502724    -0.174506     3.778838      27.32
 H       0.743623     1.472448     3.010396      25.05
 C      -0.511519    -1.164374     0.175416      21.39
 O      -1.893015    -1.104698     0.285404     141.43
 C       0.121956    -1.826582    -0.867389      71.79
 H      -0.440715    -2.431644    -1.571582      23.80
 C       2.294781    -0.884717    -0.059027      26.95
 C       3.787574    -0.694860    -0.234327      90.00
 H       4.085598    -0.587310    -1.303783      21.43
 O       4.121291     0.599272     0.421898     259.21
 H       5.036207     0.770871     0.198994      22.05
 C       4.699425    -1.803154     0.455671      75.60
 H       4.572487    -1.449047     1.554139      23.79
 O       4.311102    -3.132048     0.289318     365.42
 H       4.369922    -3.295338    -0.677729      29.61
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 C       6.189339    -1.700489     0.035690     107.38
 O       6.747446    -0.321389     0.036255     300.47
 H       7.057380    -0.193633     1.030569      26.05
 H       6.203908    -1.975225    -1.010196      31.59
 H       6.808560    -2.436324     0.552855      29.63
55
name= lig-ACN-Water-frame_6
 C      -4.208821    -0.122495    -3.047522      48.83
 H      -4.414100    -1.110444    -3.367488      18.60
 C      -3.835189     1.288586    -1.172546      65.93
 H      -3.627516     1.440013    -0.136368      24.16
 C      -3.852009     2.468043    -1.990867       7.57
 O      -3.643318     3.743928    -1.555841     204.29
 C      -3.865211     4.006876    -0.126467     109.94
 H      -3.055076     3.632630     0.517172      27.29
 H      -4.798954     3.539006     0.275509      25.61
 H      -3.957351     5.135539     0.087100      24.76
 C      -4.095023     2.314240    -3.365873       4.80
 O      -4.341442     3.310215    -4.234322     136.48
 H      -4.005610     4.277534    -3.949561      18.86
 C      -4.307425     1.013920    -3.888391      47.88
 H      -4.389957     0.869999    -5.037969      28.11
 C      -4.046300    -0.004699    -1.694899      33.64
 C      -4.163854    -1.227291    -0.709703      87.04
 H      -4.699520    -2.083997    -1.174130      28.81
 O      -4.911914    -0.917481     0.470863     147.61
 H      -4.303537    -0.466958     1.237783      22.01
 C      -2.760405    -1.985755    -0.446784      90.85
 H      -2.376667    -2.115223    -1.423941      30.63
 C      -2.860885    -3.341754     0.292860     119.10
 O      -3.338218    -4.411202    -0.554008     149.50
 H      -2.686978    -4.468324    -1.363001      28.29
 H      -3.615142    -3.346339     1.108565      27.12
 H      -1.820509    -3.650668     0.643908      25.82
 C       1.553844    -1.647433    -0.958383      60.91
 H       1.981924    -2.249506    -1.730231      23.16
 C       1.627605    -0.259380     1.014557      30.63
 H       2.337003     0.320592     1.697369      22.44
 C       0.189731    -0.419765     1.178621      20.48
 O      -0.624048     0.147476     2.117087     192.94
 C       0.031142     0.728363     3.269727     116.18
 H      -0.793152     1.196441     3.839158      26.42
 H       0.480065     0.007529     4.001391      27.02
 H       0.852191     1.404768     2.919486      27.21
 C      -0.520190    -1.166141     0.196171      22.77
 O      -1.898423    -1.101757     0.323233     156.06
 C       0.184419    -1.826031    -0.827906      76.00
 H      -0.332030    -2.380937    -1.570696      26.05
 C       2.293002    -0.938237    -0.019997      27.92
 C       3.836893    -0.664469    -0.230966     109.16
 H       4.015909    -0.630064    -1.309809      23.45
 O       4.160986     0.586594     0.449967     256.62
 H       5.000390     0.868505    -0.019917      21.13
 C       4.736958    -1.710307     0.456796      87.54
 H       4.710812    -1.652989     1.578015      23.67
 O       4.330045    -3.127542     0.259703     338.29
 H       4.115042    -3.263724    -0.714874      27.06
 C       6.180256    -1.702020    -0.059200     104.61
 O       6.752021    -0.349415    -0.004283     292.05
 H       7.223380    -0.078604     0.884512      24.95
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 H       6.249579    -2.034524    -1.071022      30.87
 H       6.759872    -2.352193     0.600565      27.87
55
name= lig-ACN-Water-frame_7
 C      -4.242165    -0.156037    -3.066612      32.38
 H      -4.327952    -1.057974    -3.626530      18.20
 C      -3.820579     1.310561    -1.132453      69.50
 H      -3.696477     1.437032    -0.089949      22.64
 C      -3.873148     2.428202    -1.985902       0.82
 O      -3.683532     3.753939    -1.534613     214.39
 C      -3.877545     4.003757    -0.134145     111.92
 H      -2.924981     3.913657     0.385468      27.66
 H      -4.641003     3.305987     0.246168      26.17
 H      -4.201813     5.047753    -0.168610      24.91
 C      -4.097160     2.278214    -3.411477      11.13
 O      -4.309324     3.330373    -4.289141      98.09
 H      -4.267465     4.285209    -3.848386      19.23
 C      -4.280016     0.962174    -3.908679      31.06
 H      -4.449754     0.807693    -5.019159      24.98
 C      -4.097624     0.002992    -1.627052      -7.77
 C      -4.167685    -1.275563    -0.772055      74.76
 H      -4.828777    -1.931936    -1.356174      25.12
 O      -4.981451    -0.911776     0.486668     145.97
 H      -4.307659    -0.632669     1.163872      26.01
 C      -2.765615    -1.963082    -0.499070      93.57
 H      -2.273312    -2.135114    -1.403073      28.39
 C      -2.917603    -3.310951     0.291680     111.16
 O      -3.329357    -4.439085    -0.584260     206.65
 H      -2.513394    -4.676539    -1.127471      27.99
 H      -3.572763    -3.093063     1.182533      25.47
 H      -1.914431    -3.549709     0.770376      25.23
 C       1.607640    -1.606841    -1.015079      39.95
 H       2.125386    -1.858618    -1.907385      21.77
 C       1.589833    -0.290405     1.019565      51.20
 H       2.067930     0.280057     1.890257      22.49
 C       0.237592    -0.484188     1.185519      18.92
 O      -0.572048     0.192564     2.137523     187.95
 C       0.054823     0.812472     3.272268     119.92
 H      -0.720984     1.409247     3.741329      26.69
 H       0.448161    -0.051082     3.900515      25.42
 H       0.798882     1.610453     3.043382      27.12
 C      -0.532843    -1.166931     0.206649      14.31
 O      -1.925858    -1.085663     0.373770     158.91
 C       0.183929    -1.811231    -0.829498      71.17
 H      -0.296303    -2.391364    -1.584085      23.09
 C       2.350080    -0.902346    -0.018876      30.18
 C       3.792674    -0.688992    -0.152689     100.86
 H       4.021755    -0.607248    -1.199293      21.90
 O       4.205901     0.650600     0.399670     224.46
 H       5.208131     0.676134     0.147512      19.46
 C       4.770549    -1.773137     0.434340      92.21
 H       4.744174    -1.490802     1.497799      25.30
 O       4.302200    -3.109070     0.216350     341.70
 H       4.434417    -3.225504    -0.802266      27.77
 C       6.230322    -1.667579    -0.101905     109.55
 O       6.771913    -0.338914    -0.064001     316.53
 H       7.089473    -0.238146     0.915096      26.77
 H       6.257185    -2.020355    -1.115390      31.66
 H       6.854349    -2.374534     0.472470      28.21
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name= lig-ACN-Water-frame_8
 C      -4.284860    -0.176547    -3.048877      66.26
 H      -4.349535    -1.237354    -3.311456      27.77
 C      -3.851609     1.288588    -1.107180      51.15
 H      -3.696364     1.423610    -0.037056      21.32
 C      -3.862570     2.406322    -2.002075       7.09
 O      -3.726508     3.729453    -1.578375     230.99
 C      -3.901358     4.039178    -0.128620     110.04
 H      -2.933521     4.112633     0.337049      30.20
 H      -4.488556     3.316561     0.426350      28.63
 H      -4.384288     4.952849    -0.011389      27.80
 C      -4.147792     2.246761    -3.422789       8.82
 O      -4.271934     3.347916    -4.326848     144.59
 H      -4.168025     4.185054    -3.853171      24.10
 C      -4.223495     0.951284    -3.935305      56.86
 H      -4.486906     0.863047    -4.992354      18.59
 C      -4.089401    -0.009778    -1.670763      23.23
 C      -4.177053    -1.210317    -0.754196      79.14
 H      -4.697100    -2.053604    -1.225433      25.70
 O      -4.965666    -0.974619     0.442580     201.47
 H      -4.436191    -0.600490     1.096903      28.22
 C      -2.811807    -1.941648    -0.492644      94.73
 H      -2.409572    -2.085683    -1.465770      27.91
 C      -2.925668    -3.299716     0.262786     108.97
 O      -3.341078    -4.416455    -0.567470     223.14
 H      -2.602312    -4.876911    -0.961971      30.24
 H      -3.839599    -3.337557     0.905257      24.24
 H      -1.978836    -3.463543     0.840522      26.36
 C       1.615038    -1.563112    -1.008930      53.51
 H       2.064530    -1.937369    -1.914326      18.84
 C       1.611179    -0.366225     1.129921      68.88
 H       2.180103     0.336536     1.787459      25.80
 C       0.190989    -0.455068     1.183181       8.87
 O      -0.505205     0.230522     2.127193     198.74
 C       0.076845     0.910991     3.314802     117.94
 H      -0.734431     1.365828     3.848314      25.71
 H       0.608949     0.197282     4.059381      25.36
 H       0.871436     1.551809     2.929698      24.06
 C      -0.535529    -1.211489     0.192719       7.81
 O      -1.939220    -1.110402     0.345481     144.21
 C       0.213603    -1.768061    -0.895333      61.90
 H      -0.349733    -2.310837    -1.659413      23.82
 C       2.293111    -0.832734    -0.012386      22.49
 C       3.856901    -0.644857    -0.170826      93.63
 H       4.024216    -0.711221    -1.222553      23.25
 O       4.261458     0.701483     0.324853     255.63
 H       5.247714     0.581266     0.363026      20.10
 C       4.781916    -1.806345     0.449233      91.03
 H       4.835774    -1.830952     1.513546      25.61
 O       4.279868    -3.105645     0.162772     357.98
 H       4.381755    -3.355836    -0.795475      29.54
 C       6.255849    -1.702745    -0.141650      99.10
 O       6.798682    -0.281169    -0.061887     260.43
 H       7.284863    -0.122749     0.804538      27.87
 H       6.223049    -1.834453    -1.223287      30.75
 H       6.972579    -2.390752     0.344401      28.71
55
name= lig-ACN-Water-frame_9
 C      -4.270074    -0.169704    -3.045109      55.93
 H      -4.544633    -1.130942    -3.566572      25.35
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 C      -3.890502     1.279352    -1.184698      64.02
 H      -3.671470     1.408630    -0.081747      23.10
 C      -3.896275     2.409835    -2.010779      25.46
 O      -3.781827     3.718561    -1.586261     205.67
 C      -3.909493     4.073188    -0.139816     120.56
 H      -2.931464     4.238724     0.266271      31.30
 H      -4.403644     3.276047     0.365109      30.18
 H      -4.411574     4.932080    -0.160942      28.67
 C      -4.136268     2.270800    -3.410906      18.54
 O      -4.229142     3.285659    -4.294953     123.28
 H      -4.002528     4.158576    -3.986234      24.28
 C      -4.247965     0.911365    -3.950911      42.51
 H      -4.276467     0.724489    -4.998108      21.95
 C      -4.073705     0.005181    -1.670031      31.42
 C      -4.167630    -1.236437    -0.728002      79.12
 H      -4.758925    -1.907531    -1.350341      24.99
 O      -4.937841    -1.033997     0.442710     214.17
 H      -4.464214    -0.354272     1.032202      25.81
 C      -2.817689    -1.946090    -0.487002      93.95
 H      -2.401221    -2.112795    -1.483278      27.48
 C      -3.012683    -3.307861     0.256788     117.03
 O      -3.360574    -4.420263    -0.568789     233.91
 H      -2.557933    -4.568086    -1.165893      28.46
 H      -3.679298    -3.058261     1.106744      25.69
 H      -2.064561    -3.592947     0.759293      26.54
 C       1.578793    -1.510487    -0.985501      48.09
 H       2.178102    -2.011515    -1.769367      21.38
 C       1.643090    -0.395456     1.167019      51.80
 H       2.169781     0.131016     1.949028      27.49
 C       0.232896    -0.427148     1.197587      -9.12
 O      -0.536560     0.276370     2.183678     181.25
 C       0.145185     0.964206     3.289926     114.06
 H      -0.712495     1.439926     3.749110      25.89
 H       0.622548     0.178885     3.986900      25.06
 H       0.753668     1.824873     3.047117      26.18
 C      -0.519239    -1.186659     0.187685       4.04
 O      -1.895166    -1.133295     0.275262     143.79
 C       0.175214    -1.704977    -0.923688      72.92
 H      -0.264427    -2.258863    -1.793053      24.34
 C       2.351792    -0.821308    -0.002775      21.12
 C       3.875997    -0.622187    -0.203291      92.71
 H       4.083654    -0.644734    -1.246495      23.58
 O       4.309808     0.707532     0.248402     265.30
 H       5.260475     0.705553     0.123824      22.98
 C       4.824381    -1.793284     0.449206      85.11
 H       4.787229    -1.633661     1.478991      26.70
 O       4.265965    -3.149743     0.112538     362.61
 H       4.153704    -3.035192    -0.858690      28.04
 C       6.254460    -1.637857    -0.181170      99.61
 O       6.825427    -0.250906    -0.011440     245.19
 H       7.253250    -0.261254     0.888409      25.56
 H       6.183197    -1.920256    -1.260702      30.50
 H       6.924656    -2.406344     0.271519      29.23
55
name= lig-ACN-Water-frame_10
 C      -4.268995    -0.185779    -3.093379      41.25
 H      -4.378617    -1.248041    -3.492495      22.65
 C      -3.877428     1.311460    -1.186933      43.13
 H      -3.716640     1.510142    -0.056531      20.78
 C      -3.971029     2.426063    -2.026027      11.91
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 O      -3.819527     3.753191    -1.578044     223.62
 C      -3.915948     4.090490    -0.201972     131.56
 H      -2.932818     4.244407     0.196821      28.73
 H      -4.457223     3.412842     0.401603      28.33
 H      -4.416020     4.946234    -0.150331      27.37
 C      -4.087386     2.186208    -3.421530      30.15
 O      -4.177396     3.261966    -4.310594     136.28
 H      -4.155206     4.128192    -3.764470      21.46
 C      -4.260031     0.956427    -3.915551      85.81
 H      -4.343878     0.864478    -4.967832      27.36
 C      -4.091571    -0.050589    -1.675573      -9.93
 C      -4.150511    -1.262919    -0.802685      74.97
 H      -4.741400    -2.065830    -1.240995      25.53
 O      -4.925427    -1.060419     0.501279     104.50
 H      -4.429402    -0.350179     1.150701      23.36
 C      -2.775465    -2.017544    -0.545806      78.11
 H      -2.310863    -2.320470    -1.528632      27.05
 C      -2.995217    -3.291933     0.316239     106.79
 O      -3.414645    -4.427620    -0.600094     119.69
 H      -2.759255    -4.470744    -1.377334      29.39
 H      -3.820807    -3.318273     1.012097      25.29
 H      -2.021150    -3.483071     0.790990      26.38
 C       1.620671    -1.477457    -0.978232      58.72
 H       2.052926    -1.776932    -1.980118      22.12
 C       1.670162    -0.356293     1.163714      58.18
 H       2.166552    -0.032227     2.026169      24.89
 C       0.245710    -0.414831     1.232134      -4.88
 O      -0.529674     0.273793     2.178430     194.91
 C       0.132618     1.012926     3.263419     113.40
 H      -0.586039     1.412119     3.987963      25.97
 H       0.809904     0.284140     3.848863      24.41
 H       0.839726     1.669200     2.792176      27.47
 C      -0.493294    -1.076034     0.177487       0.33
 O      -1.883064    -1.095568     0.269064     119.91
 C       0.213230    -1.639600    -0.897707      70.30
 H      -0.411777    -2.194060    -1.655208      25.11
 C       2.392200    -0.855781     0.033087      12.74
 C       3.881207    -0.670154    -0.232618     127.87
 H       3.959935    -0.751560    -1.291995      23.43
 O       4.326216     0.705183     0.185462     274.61
 H       5.248968     0.739211    -0.173222      20.68
 C       4.781935    -1.742145     0.363946     106.68
 H       4.835874    -1.689965     1.399803      28.69
 O       4.299955    -3.079793     0.106849     313.94
 H       4.320621    -3.304613    -0.851605      30.16
 C       6.245006    -1.586685    -0.166262      98.67
 O       6.849869    -0.276845     0.036536     284.02
 H       7.157343    -0.120832     0.982927      25.33
 H       6.267926    -1.614388    -1.300988      29.00
 H       6.946487    -2.349105     0.272351      28.23
55
name= lig-ACN-Water-frame_11
 C      -4.257017    -0.232067    -3.070552      54.72
 H      -4.269197    -1.260932    -3.505765      24.17
 C      -3.900315     1.254222    -1.149467      55.29
 H      -3.791324     1.336346    -0.009438      19.24
 C      -3.979321     2.418027    -1.979952      20.34
 O      -3.868882     3.762417    -1.658596     245.83
 C      -3.938363     4.140101    -0.190759     118.89
 H      -2.945801     4.121830     0.229120      28.67
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 H      -4.499014     3.411011     0.320209      28.35
 H      -4.293723     5.094805    -0.139476      25.96
 C      -4.086707     2.272105    -3.410055       0.12
 O      -4.114921     3.260033    -4.323602      57.75
 H      -4.207280     4.277872    -3.987927      21.87
 C      -4.254717     0.880471    -3.963338      23.29
 H      -4.517110     0.810517    -5.021728      21.19
 C      -4.100081    -0.004113    -1.710893      35.07
 C      -4.142459    -1.322170    -0.751539      73.55
 H      -4.738289    -2.025728    -1.345329      25.03
 O      -4.870685    -1.085645     0.482563     202.03
 H      -4.192522    -0.760319     1.168104      23.51
 C      -2.743347    -2.020101    -0.499227      82.18
 H      -2.241291    -2.224817    -1.518468      25.16
 C      -2.946366    -3.371871     0.276443     119.38
 O      -3.447139    -4.394448    -0.609546     184.96
 H      -2.718971    -4.684210    -1.180313      29.02
 H      -3.731202    -3.069405     0.957290      26.71
 H      -2.121182    -3.739523     0.880452      26.63
 C       1.652465    -1.445603    -1.016542      47.07
 H       2.198470    -1.713087    -1.964894      20.84
 C       1.685867    -0.343112     1.186715      61.52
 H       2.286194     0.204181     1.859040      21.50
 C       0.247580    -0.359274     1.234543      15.06
 O      -0.534728     0.244548     2.185606     210.64
 C       0.200868     0.993301     3.202731     116.07
 H      -0.656743     1.462292     3.761561      24.05
 H       0.850607     0.343455     3.840615      25.43
 H       0.669899     1.885805     2.808532      25.92
 C      -0.490734    -0.993757     0.182849      20.09
 O      -1.908022    -1.046081     0.260312     189.07
 C       0.271817    -1.585181    -0.839139      69.97
 H      -0.208329    -2.068025    -1.718283      19.48
 C       2.346622    -0.876933     0.043678      31.86
 C       3.839871    -0.658513    -0.288359      99.30
 H       3.946710    -0.742253    -1.355736      20.43
 O       4.296609     0.673400     0.104882     262.29
 H       5.299843     0.763121    -0.096445      19.46
 C       4.812953    -1.706506     0.340041     100.65
 H       4.726462    -1.524735     1.373565      25.99
 O       4.347753    -3.030687     0.121343     362.71
 H       4.573928    -3.185511    -0.833165      28.92
 C       6.269083    -1.559959    -0.176686      91.60
 O       6.882329    -0.255247     0.072456     336.23
 H       7.332931    -0.223441     1.018555      25.69
 H       6.237237    -1.773664    -1.300490      30.62
 H       6.797940    -2.458133     0.253211      28.64
55
name= lig-ACN-Water-frame_12
 C      -4.222512    -0.207590    -3.093254      56.04
 H      -4.417267    -1.178762    -3.519451      26.90
 C      -3.966600     1.264231    -1.120963      38.60
 H      -3.847627     1.373249    -0.021900      21.01
 C      -3.941860     2.394727    -2.006242       9.59
 O      -3.921130     3.789666    -1.643483     185.82
 C      -3.940479     4.138639    -0.235312     125.58
 H      -2.970418     3.972554     0.212320      30.42
 H      -4.738358     3.653556     0.276746      30.30
 H      -4.175892     5.196564    -0.244466      26.91
 C      -4.136215     2.165965    -3.423803      13.50
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 O      -4.064940     3.278842    -4.371454      59.78
 H      -3.971185     4.172022    -3.837631      20.43
 C      -4.248085     0.918669    -3.929605      95.12
 H      -4.267131     0.711147    -5.029696      22.42
 C      -4.069854    -0.104462    -1.641927     -22.58
 C      -4.091556    -1.314033    -0.763765      66.44
 H      -4.686894    -2.103228    -1.270445      23.74
 O      -4.798995    -1.124499     0.465826     191.54
 H      -4.267823    -0.748702     1.126227      26.16
 C      -2.673802    -1.971025    -0.475687      83.64
 H      -2.235338    -2.137144    -1.544609      25.35
 C      -2.913739    -3.375563     0.270437     113.67
 O      -3.447632    -4.381337    -0.628187     204.08
 H      -2.694332    -4.897272    -0.962127      29.12
 H      -3.627519    -3.342025     1.095292      25.68
 H      -1.949758    -3.699943     0.648331      26.40
 C       1.628108    -1.430189    -0.994742      50.09
 H       2.127454    -1.945998    -1.830999      21.42
 C       1.674082    -0.317341     1.157869      60.72
 H       2.138297     0.361851     1.875803      21.53
 C       0.260633    -0.326314     1.190256      14.52
 O      -0.509392     0.225329     2.220907     223.13
 C       0.184529     1.035183     3.184500     117.27
 H      -0.570045     1.390404     3.950932      24.32
 H       0.867941     0.372174     3.747383      26.50
 H       0.828968     1.786879     2.703464      25.52
 C      -0.486574    -1.026366     0.178751      13.33
 O      -1.899137    -0.994900     0.271848     168.29
 C       0.226052    -1.574985    -0.914508      59.95
 H      -0.360714    -2.066524    -1.674535      22.86
 C       2.399233    -0.806058     0.019916      39.57
 C       3.834457    -0.630919    -0.335655     101.74
 H       3.905000    -0.737713    -1.421546      20.65
 O       4.247403     0.700738     0.043321     274.76
 H       5.240066     0.583415     0.111506      19.41
 C       4.823540    -1.624206     0.378330      87.67
 H       4.887433    -1.454962     1.438868      23.62
 O       4.417569    -3.039062     0.130409     346.28
 H       4.226634    -3.148978    -0.865874      26.95
 C       6.288316    -1.577435    -0.173517      97.51
 O       6.920769    -0.247748     0.052695     304.81
 H       7.318546    -0.219175     1.047130      25.35
 H       6.344894    -1.674938    -1.296033      29.14
 H       6.983109    -2.286383     0.339273      28.10
55
name= lig-ACN-Water-frame_13
 C      -4.210334    -0.228663    -3.017371      70.75
 H      -4.269845    -1.183917    -3.444971      26.84
 C      -3.999975     1.268577    -1.152563      69.18
 H      -3.978642     1.534100    -0.125406      24.51
 C      -3.981734     2.376116    -2.027802      18.85
 O      -3.954798     3.729175    -1.649578     214.42
 C      -3.959996     4.148634    -0.272470     118.19
 H      -3.104575     3.748734     0.278572      30.18
 H      -4.817798     3.790989     0.284268      27.88
 H      -3.841927     5.277901    -0.259901      25.95
 C      -4.096829     2.257596    -3.448324       3.25
 O      -4.024406     3.201221    -4.342009      68.57
 H      -4.034608     4.125982    -4.034703      22.50
 C      -4.216674     0.878464    -3.923658      21.79
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 H      -4.189983     0.796242    -5.058345      21.29
 C      -4.050783    -0.041158    -1.672879      32.56
 C      -4.015713    -1.349523    -0.767823      68.65
 H      -4.527378    -2.171682    -1.325785      23.99
 O      -4.776110    -1.158001     0.502198     167.56
 H      -4.356127    -0.455164     1.031966      25.64
 C      -2.689593    -1.951390    -0.489850      89.14
 H      -2.108873    -2.268857    -1.431343      24.98
 C      -2.784054    -3.322330     0.263126     106.44
 O      -3.419337    -4.369680    -0.645401     176.27
 H      -2.676651    -4.848798    -1.169005      28.07
 H      -3.389250    -3.243970     1.183372      25.58
 H      -1.762103    -3.621878     0.505660      26.76
 C       1.570112    -1.488335    -0.975938      56.77
 H       2.078144    -1.894144    -1.830307      18.29
 C       1.670935    -0.207235     1.074058      50.63
 H       2.308216     0.168959     1.934346      23.35
 C       0.249136    -0.352050     1.175053       7.00
 O      -0.500999     0.207463     2.211680     184.41
 C       0.219019     1.033054     3.235294     108.56
 H      -0.573011     1.550548     3.862854      25.26
 H       0.934529     0.465377     3.807502      26.59
 H       0.679482     1.908439     2.704932      26.59
 C      -0.496575    -1.056029     0.168848      14.87
 O      -1.855535    -0.975837     0.304565     135.28
 C       0.162755    -1.617790    -0.940330      74.85
 H      -0.257220    -2.212215    -1.698740      26.46
 C       2.333486    -0.758671    -0.044823      24.34
 C       3.898135    -0.619852    -0.307995      94.31
 H       4.051210    -0.796896    -1.394107      24.21
 O       4.251979     0.783798     0.015771     306.05
 H       5.200163     0.881287     0.019922      22.77
 C       4.860331    -1.674387     0.341264      97.73
 H       4.737666    -1.533340     1.431321      25.73
 O       4.457717    -3.016975     0.161865     358.31
 H       4.294148    -3.160181    -0.826598      28.64
 C       6.340707    -1.526802    -0.144971      93.03
 O       6.943160    -0.217465     0.003390     293.29
 H       7.225350    -0.081915     1.026313      24.40
 H       6.310555    -1.786730    -1.228021      30.77
 H       6.815940    -2.427745     0.316351      29.27
55
name= lig-ACN-Water-frame_14
 C      -4.178306    -0.232807    -3.063347      51.52
 H      -4.084723    -1.207183    -3.444236      33.70
 C      -4.011211     1.320526    -1.152940      61.37
 H      -4.024284     1.388866    -0.116117      25.18
 C      -4.069321     2.399409    -2.029129      21.91
 O      -3.978007     3.708589    -1.674282     208.55
 C      -3.952352     4.117016    -0.250840     103.26
 H      -3.207546     3.537156     0.301611      28.10
 H      -4.987358     4.083641     0.128726      24.45
 H      -3.667667     5.268636    -0.359770      23.44
 C      -4.031350     2.131035    -3.406579      24.37
 O      -3.984614     3.215641    -4.401036     138.88
 H      -4.025807     4.068330    -3.967467      25.24
 C      -4.149781     0.869211    -3.909500      68.41
 H      -4.355638     0.646534    -4.982310      22.23
 C      -4.051387    -0.045709    -1.623651     -23.73
 C      -4.056547    -1.288148    -0.734914      73.94
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 H      -4.696155    -1.992203    -1.322573      22.15
 O      -4.780201    -1.204453     0.483664     177.21
 H      -4.349814    -0.510143     1.201686      22.50
 C      -2.607331    -1.965044    -0.487539      88.57
 H      -2.218286    -1.917967    -1.547963      26.68
 C      -2.648674    -3.326186     0.202188     119.70
 O      -3.336422    -4.302446    -0.611592     240.47
 H      -2.669729    -4.451697    -1.327962      29.94
 H      -3.237080    -3.188771     1.148660      24.57
 H      -1.648501    -3.704297     0.484161      25.52
 C       1.583154    -1.538581    -1.045228      46.39
 H       2.067845    -1.953042    -1.893385      24.82
 C       1.656210    -0.152026     0.990188      48.35
 H       2.258517     0.377295     1.823097      23.06
 C       0.286813    -0.342885     1.192742      11.14
 O      -0.479394     0.197862     2.227784     184.03
 C       0.210588     1.029956     3.222004     114.20
 H      -0.674109     1.304540     3.835726      26.00
 H       0.859416     0.455827     3.857260      27.28
 H       0.809177     1.886212     2.783971      27.90
 C      -0.484146    -1.030026     0.170588       4.66
 O      -1.892045    -1.016448     0.331588     145.16
 C       0.184068    -1.705858    -0.884566      71.52
 H      -0.380321    -2.212877    -1.622181      24.41
 C       2.337573    -0.752460    -0.120982      20.40
 C       3.875246    -0.592596    -0.319362     104.10
 H       4.039882    -0.632910    -1.430328      21.64
 O       4.272994     0.833031     0.029108     282.79
 H       5.169907     0.865183    -0.411950      24.32
 C       4.878164    -1.645552     0.396163      88.61
 H       4.942061    -1.466897     1.517903      25.12
 O       4.449544    -3.033482     0.148822     308.53
 H       4.674536    -3.233536    -0.783349      30.59
 C       6.339011    -1.532734    -0.146012     109.66
 O       6.969570    -0.170804    -0.022007     257.22
 H       7.395468    -0.214743     0.917608      25.25
 H       6.410618    -1.722353    -1.215955      30.43
 H       7.086901    -2.102973     0.418728      27.52
55
name= lig-ACN-Water-frame_15
 C      -4.078419    -0.272259    -3.004210      49.96
 H      -4.179880    -1.259252    -3.439170      19.00
 C      -4.051979     1.263344    -1.085807      61.42
 H      -4.027757     1.546320    -0.067916      21.77
 C      -4.083414     2.382837    -2.023344      -1.78
 O      -3.999239     3.770921    -1.674166     222.75
 C      -3.964065     4.100286    -0.289098     103.19
 H      -3.389259     3.390049     0.356802      26.59
 H      -4.973369     4.108685     0.244489      24.37
 H      -3.406703     5.176286    -0.157424      23.52
 C      -4.008380     2.177170    -3.502710       5.68
 O      -3.954346     3.164409    -4.390324     148.89
 H      -3.724314     4.078321    -4.004811      21.95
 C      -4.096876     0.806418    -3.949569      48.39
 H      -4.086372     0.705711    -5.039425      27.82
 C      -4.065781    -0.029025    -1.634109      49.53
 C      -4.074995    -1.288950    -0.720112      94.20
 H      -4.520415    -2.150063    -1.286694      26.65
 O      -4.845696    -1.224155     0.505572     172.12
 H      -4.263670    -0.809072     1.310311      21.23
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 C      -2.629750    -1.880800    -0.558559      88.40
 H      -2.129954    -2.024342    -1.528907      28.55
 C      -2.554731    -3.312046     0.172894     115.07
 O      -3.247508    -4.259089    -0.617227     221.19
 H      -2.738691    -4.534291    -1.379033      31.25
 H      -3.136512    -3.300798     1.144009      25.91
 H      -1.480515    -3.577139     0.360018      26.22
 C       1.628837    -1.555802    -1.092207      51.78
 H       2.084188    -2.131813    -1.876569      23.37
 C       1.683803    -0.154799     0.920054      66.53
 H       2.226867     0.670783     1.479017      25.88
 C       0.279491    -0.301952     1.150291      20.67
 O      -0.435828     0.187685     2.221001     202.25
 C       0.159396     0.980866     3.250512     122.68
 H      -0.548991     1.482574     3.907618      26.75
 H       0.859579     0.362187     3.791177      27.18
 H       0.716953     1.835312     2.763543      26.73
 C      -0.469228    -1.033970     0.207042      18.18
 O      -1.861893    -1.048600     0.370608     147.09
 C       0.233993    -1.730878    -0.812296      65.49
 H      -0.324543    -2.380848    -1.495831      24.83
 C       2.371256    -0.764595    -0.158445      18.86
 C       3.855980    -0.541359    -0.350549     100.49
 H       4.075870    -0.790270    -1.440644      22.30
 O       4.289512     0.800161     0.045319     281.12
 H       5.108534     1.035950    -0.482451      23.52
 C       4.868283    -1.599134     0.387358      73.13
 H       4.760973    -1.476740     1.545285      24.69
 O       4.454827    -3.014193     0.152174     313.84
 H       4.654087    -3.208594    -0.798130      28.88
 C       6.389079    -1.478259    -0.141782      94.64
 O       6.990885    -0.129227    -0.038873     312.93
 H       7.449729    -0.017825     0.820766      25.08
 H       6.373349    -1.802952    -1.168810      30.26
 H       6.848943    -2.318536     0.382731      27.93
55
name= lig-ACN-Water-frame_16
 C      -4.024530    -0.236705    -3.013396      45.41
 H      -3.942951    -1.322694    -3.331196      29.39
 C      -4.107036     1.322737    -1.133077      59.96
 H      -4.189499     1.359168    -0.036899      23.97
 C      -4.027610     2.393876    -2.048714      25.23
 O      -4.025315     3.746587    -1.707368     182.56
 C      -3.957930     4.081358    -0.237631      90.77
 H      -3.348061     3.255767     0.247044      29.10
 H      -5.059185     4.185406     0.106530      25.85
 H      -3.423833     5.180246    -0.179483      24.66
 C      -4.023058     2.121664    -3.417967       9.91
 O      -3.906537     3.160818    -4.415194      82.43
 H      -3.801316     4.127310    -3.950044      22.83
 C      -3.990262     0.805838    -3.945681      85.86
 H      -3.843957     0.534583    -4.957575      26.89
 C      -4.098433    -0.064350    -1.580687     -56.19
 C      -4.053128    -1.359639    -0.726483      78.03
 H      -4.613825    -2.102521    -1.348365      22.70
 O      -4.886189    -1.235952     0.522503     189.06
 H      -4.358047    -0.688854     1.169684      26.88
 C      -2.637007    -1.880164    -0.488597      88.92
 H      -2.246110    -1.810429    -1.488846      27.94
 C      -2.532672    -3.219966     0.112995     116.17
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 O      -3.216135    -4.302717    -0.677207     266.57
 H      -2.400258    -4.699666    -1.140165      27.87
 H      -2.878726    -3.164628     1.194469      25.34
 H      -1.438479    -3.458560     0.168515      25.18
 C       1.646791    -1.585590    -1.014712      51.04
 H       2.140449    -2.098073    -1.857111      22.65
 C       1.700609    -0.097518     0.872932      45.03
 H       2.289422     0.545589     1.535246      25.57
 C       0.323901    -0.257346     1.111100       5.44
 O      -0.468451     0.180701     2.196772     182.66
 C       0.208060     0.964141     3.276633     113.55
 H      -0.691688     1.220137     3.791795      26.13
 H       0.857571     0.381000     3.934256      26.44
 H       0.722085     1.859901     2.868874      26.01
 C      -0.427238    -1.088021     0.206947      11.69
 O      -1.790392    -1.033958     0.385047     143.24
 C       0.271304    -1.739626    -0.814271      78.55
 H      -0.200218    -2.550504    -1.440059      24.77
 C       2.391024    -0.755017    -0.197480      20.03
 C       3.937114    -0.605559    -0.400946     119.43
 H       4.122281    -0.530595    -1.530238      23.40
 O       4.269093     0.788069     0.043604     294.18
 H       5.177194     0.877328    -0.240492      21.88
 C       4.831291    -1.579880     0.312020      86.07
 H       4.716684    -1.339296     1.464940      24.16
 O       4.482155    -2.934964     0.156046     342.35
 H       4.338372    -3.108471    -0.831939      28.69
 C       6.333943    -1.431634    -0.099502     105.24
 O       7.018248    -0.127112    -0.056037     319.35
 H       7.433664    -0.147401     0.810319      26.72
 H       6.391256    -1.620366    -1.146544      29.42
 H       7.030551    -2.055315     0.431863      26.95
55
name= lig-ACN-Water-frame_17
 C      -3.983841    -0.281683    -2.972836      72.44
 H      -3.713890    -1.273262    -3.456316      25.66
 C      -4.167649     1.273702    -1.145713      74.89
 H      -4.351734     1.649868    -0.098332      23.45
 C      -4.021316     2.387232    -2.026354       7.81
 O      -4.028713     3.721086    -1.689451     191.39
 C      -3.961782     4.047945    -0.278282     101.96
 H      -3.305731     3.389409     0.436125      26.88
 H      -5.014983     4.046765     0.268550      25.32
 H      -3.491943     5.139630    -0.266563      25.06
 C      -3.963607     2.138667    -3.481570      15.04
 O      -3.871856     3.129780    -4.388971      79.08
 H      -3.943315     4.082025    -3.961274      24.85
 C      -3.876662     0.814518    -3.870405      44.01
 H      -3.846338     0.726589    -4.921860      18.82
 C      -4.116865    -0.038808    -1.612029      21.51
 C      -4.119485    -1.297338    -0.668055      82.31
 H      -4.518956    -2.195949    -1.198705      23.97
 O      -4.855298    -1.221195     0.497358     173.58
 H      -4.491240    -0.604569     1.076818      28.76
 C      -2.593156    -1.817707    -0.499998      86.26
 H      -2.155682    -1.883066    -1.460200      28.16
 C      -2.530803    -3.304090     0.081190     118.15
 O      -3.172312    -4.303045    -0.687038     259.05
 H      -2.506890    -4.888280    -1.180935      27.47
 H      -3.025608    -3.343111     1.098425      25.46
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 H      -1.436452    -3.537126     0.174595      25.13
 C       1.688058    -1.632608    -0.980246      52.47
 H       2.181746    -2.159824    -1.845768      21.88
 C       1.751346    -0.021427     0.888758      48.22
 H       2.280450     0.442416     1.664899      26.79
 C       0.353379    -0.263632     1.100757       6.70
 O      -0.412285     0.206371     2.157831     185.24
 C       0.172156     0.934914     3.276168     118.02
 H      -0.553324     1.252002     3.995906      26.94
 H       0.883186     0.219489     3.749883      25.60
 H       0.713255     1.820456     2.950950      27.91
 C      -0.371708    -1.083422     0.180361       7.35
 O      -1.778652    -1.005436     0.385366     141.96
 C       0.273893    -1.818752    -0.856059      68.65
 H      -0.378320    -2.410619    -1.576984      23.45
 C       2.442443    -0.710500    -0.177545      12.70
 C       3.905583    -0.530485    -0.489203     112.76
 H       4.132657    -0.783512    -1.596719      23.45
 O       4.263747     0.770110     0.038213     284.72
 H       5.228401     0.857988     0.210118      19.50
 C       4.864054    -1.519004     0.314471      80.92
 H       4.741119    -1.301697     1.469771      24.56
 O       4.471907    -2.912284     0.128942     336.14
 H       4.401411    -3.101935    -0.857582      27.48
 C       6.340886    -1.422689    -0.137482     103.42
 O       7.018887    -0.104271    -0.028255     305.06
 H       7.610643    -0.079704     0.793152      27.24
 H       6.391592    -1.842196    -1.118351      31.35
 H       6.748209    -2.196095     0.493737      28.54
55
name= lig-ACN-Water-frame_18
 C      -3.902123    -0.299616    -2.996698      33.09
 H      -3.923381    -1.377410    -3.303072      22.40
 C      -4.231713     1.291312    -1.142922      52.76
 H      -4.423550     1.373871    -0.038204      19.98
 C      -4.069758     2.346902    -2.056319      29.42
 O      -4.013807     3.684238    -1.648844     217.33
 C      -3.966748     4.066582    -0.271212      95.37
 H      -3.089011     3.411446     0.170349      26.22
 H      -5.029896     3.861938     0.227756      22.57
 H      -3.735765     5.188927    -0.221277      23.82
 C      -3.860561     2.160388    -3.394922      18.75
 O      -3.852902     3.139028    -4.401551     152.42
 H      -3.682793     4.067994    -4.107849      20.96
 C      -3.847132     0.796287    -3.889916      43.98
 H      -3.721670     0.556926    -4.931025      33.04
 C      -4.141360    -0.067835    -1.599607      -5.08
 C      -4.023354    -1.261424    -0.710468      99.31
 H      -4.565600    -2.030807    -1.302173      26.69
 O      -4.853206    -1.146399     0.528188     194.89
 H      -4.337201    -0.727680     1.248317      25.05
 C      -2.599796    -1.841027    -0.525847      85.69
 H      -2.220831    -1.793944    -1.509339      31.15
 C      -2.531998    -3.360608     0.129729     115.40
 O      -3.212097    -4.332243    -0.717664     261.94
 H      -2.548002    -4.525049    -1.415746      29.97
 H      -3.096846    -3.276053     1.082294      26.22
 H      -1.474886    -3.610287     0.420179      25.72
 C       1.709328    -1.631818    -0.983911      48.44
 H       2.313401    -2.199466    -1.744169      20.96
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 C       1.788125    -0.045533     0.924545      80.70
 H       2.314249     0.689701     1.439114      30.09
 C       0.418754    -0.276440     1.109741      -0.64
 O      -0.389227     0.261864     2.105132     190.88
 C       0.213049     0.873571     3.259287     113.99
 H      -0.665542     1.060487     3.871917      26.30
 H       0.962661     0.225504     3.792575      25.47
 H       0.657801     1.813839     2.970745      27.25
 C      -0.383430    -1.051492     0.143450       6.41
 O      -1.755480    -0.982861     0.349854     139.53
 C       0.311137    -1.799971    -0.831798      69.80
 H      -0.128875    -2.411244    -1.655935      24.53
 C       2.385420    -0.724921    -0.182837      34.31
 C       3.912843    -0.491353    -0.437631     116.07
 H       4.069635    -0.429081    -1.580224      22.02
 O       4.267162     0.827067     0.016323     268.36
 H       5.305104     0.819694    -0.024377      19.82
 C       4.841475    -1.494392     0.257596      78.34
 H       4.749334    -1.297504     1.407738      24.27
 O       4.451820    -2.896871     0.094483     347.12
 H       4.721578    -3.142695    -0.812569      30.15
 C       6.381295    -1.477292    -0.139687     108.99
 O       7.009435    -0.124908     0.007122     296.16
 H       7.530296    -0.290015     0.902933      25.58
 H       6.529122    -1.643120    -1.195833      29.60
 H       7.001431    -2.130949     0.450575      27.78
55
name= lig-ACN-Water-frame_19
 C      -3.920655    -0.269896    -2.998617      64.85
 H      -3.827216    -1.264012    -3.433845      20.48
 C      -4.277949     1.249296    -1.128457      75.72
 H      -4.485687     1.435426    -0.075182      24.12
 C      -4.099439     2.366635    -1.966597      -4.66
 O      -4.012052     3.700639    -1.669895     178.39
 C      -3.969852     4.047444    -0.232651     108.18
 H      -3.005944     3.708280     0.379659      26.92
 H      -4.890669     3.637394     0.382358      24.06
 H      -3.970797     5.132054    -0.246060      26.08
 C      -3.820545     2.085358    -3.459183      -9.82
 O      -3.804222     3.135392    -4.408532     136.80
 H      -3.644845     4.028841    -4.095401      20.08
 C      -3.882331     0.782791    -3.923978      79.87
 H      -3.715365     0.664192    -5.014117      28.92
 C      -4.071003    -0.047975    -1.633954      40.72
 C      -4.026115    -1.302777    -0.680716      85.39
 H      -4.511794    -2.156712    -1.173595      26.09
 O      -4.823326    -1.077513     0.498512     180.37
 H      -4.263930    -0.625683     1.268160      20.86
 C      -2.561566    -1.941039    -0.505739      90.43
 H      -2.123025    -2.082937    -1.475715      28.03
 C      -2.634685    -3.286575     0.159342     117.55
 O      -3.251357    -4.335110    -0.736675     217.29
 H      -2.648949    -4.486076    -1.482811      30.87
 H      -3.229053    -3.294232     1.069351      26.21
 H      -1.611222    -3.667484     0.326395      25.85
 C       1.730196    -1.610320    -0.988048      59.58
 H       2.202151    -2.218159    -1.779605      21.61
 C       1.776863    -0.100645     0.895830      64.56
 H       2.271380     0.686410     1.438135      30.94
 C       0.381707    -0.290733     1.086612      16.75
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 O      -0.379582     0.305511     2.046429     206.37
 C       0.244638     0.857554     3.254920     113.73
 H      -0.575305     0.936905     4.010185      26.42
 H       0.988211     0.119155     3.689346      25.36
 H       0.697951     1.825588     3.139561      26.98
 C      -0.334251    -1.025483     0.153973       4.35
 O      -1.751068    -0.977997     0.279400     138.73
 C       0.345664    -1.746163    -0.849541      77.86
 H      -0.251733    -2.488084    -1.342750      26.33
 C       2.473097    -0.720503    -0.148597      21.90
 C       3.895599    -0.463666    -0.437673     114.39
 H       4.046678    -0.564966    -1.569263      22.07
 O       4.307492     0.941847     0.030253     287.92
 H       5.181858     1.124157    -0.379985      20.81
 C       4.893177    -1.576801     0.220706      81.52
 H       4.806013    -1.337992     1.345035      24.35
 O       4.431826    -2.885120     0.052716     351.34
 H       4.595242    -3.235549    -0.869087      29.45
 C       6.401575    -1.454763    -0.169974      92.40
 O       7.003645    -0.173900     0.068459     339.38
 H       7.459245    -0.078004     1.002486      24.45
 H       6.428828    -1.730032    -1.238496      29.20
 H       6.859643    -2.302091     0.338073      27.97
55
name= lig-ACN-Water-frame_20
 C      -3.952917    -0.301413    -3.050730      61.11
 H      -3.727752    -1.298509    -3.382786      32.59
 C      -4.255369     1.255885    -1.121390      57.99
 H      -4.517729     1.448053    -0.111730      27.71
 C      -4.044182     2.324506    -2.080341      18.01
 O      -4.015181     3.725183    -1.624565     181.99
 C      -3.995044     4.062278    -0.202976     112.30
 H      -2.907218     3.802731     0.154359      28.27
 H      -4.804714     3.455521     0.363359      26.62
 H      -4.209857     5.080632    -0.108355      28.33
 C      -3.926041     2.154676    -3.427586      26.21
 O      -3.730539     3.071712    -4.388706     133.08
 H      -3.723462     4.010952    -4.088449      24.50
 C      -3.931425     0.811341    -3.961797      38.40
 H      -3.947249     0.601751    -5.081349      17.11
 C      -4.015642    -0.105123    -1.619564     -34.19
 C      -4.036419    -1.341104    -0.719698      79.41
 H      -4.616916    -2.115247    -1.210764      24.01
 O      -4.787309    -1.049524     0.472106     160.64
 H      -4.206217    -0.383341     1.102524      23.06
 C      -2.599633    -1.930319    -0.503095      89.35
 H      -2.224252    -2.098440    -1.519090      28.57
 C      -2.728352    -3.356399     0.178901     120.92
 O      -3.314994    -4.273159    -0.728219     235.03
 H      -2.529470    -4.710219    -1.209573      27.79
 H      -3.360022    -3.289936     1.046544      26.89
 H      -1.749887    -3.627832     0.611005      26.62
 C       1.776694    -1.582539    -1.016375      46.15
 H       2.287185    -2.082559    -1.822078      21.07
 C       1.765661    -0.090680     0.898604      32.37
 H       2.293529     0.424450     1.745431      24.29
 C       0.376745    -0.245275     1.059173     -10.99
 O      -0.402199     0.396313     2.053064     208.01
 C       0.266639     0.810331     3.269278     109.42
 H      -0.498581     0.922688     4.100941      25.44
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 H       1.076739     0.053249     3.491756      24.59
 H       0.710672     1.789950     3.059095      25.53
 C      -0.376743    -1.057843     0.132699       9.84
 O      -1.734969    -1.006625     0.208428     156.32
 C       0.350627    -1.736848    -0.851362      81.89
 H      -0.056554    -2.425395    -1.535538      26.73
 C       2.494457    -0.741525    -0.155861       3.76
 C       4.024217    -0.440822    -0.440198     115.18
 H       4.170628    -0.448205    -1.561882      21.82
 O       4.308704     0.992772    -0.008056     285.44
 H       5.163242     1.167697    -0.389552      23.25
 C       4.925309    -1.528939     0.254411      94.10
 H       4.892347    -1.460416     1.365051      24.17
 O       4.396913    -2.933434    -0.004054     367.02
 H       4.413645    -3.021811    -1.026159      27.43
 C       6.372064    -1.492303    -0.230128     105.95
 O       7.002494    -0.181521     0.102685     291.77
 H       7.566729    -0.334873     0.905461      25.96
 H       6.559404    -1.590840    -1.326275      29.53
 H       6.974711    -2.247061     0.291346      28.42
55
name= lig-ACN-Water-frame_21
 C      -3.937776    -0.296954    -3.058973      83.37
 H      -3.997534    -1.280771    -3.493798      21.86
 C      -4.136565     1.231954    -1.230586      81.27
 H      -4.269917     1.329303    -0.179202      24.94
 C      -4.033843     2.386712    -1.981994       2.97
 O      -4.026470     3.687519    -1.628664     191.34
 C      -4.012563     4.024072    -0.198019     128.66
 H      -2.954278     3.954152     0.265387      27.95
 H      -4.672386     3.390207     0.429043      27.80
 H      -4.324011     5.014725    -0.147790      27.71
 C      -4.008326     2.094531    -3.458303     -11.84
 O      -3.666163     3.095256    -4.414298     -19.22
 H      -3.512892     4.073575    -4.042423      23.03
 C      -4.013406     0.776963    -3.900434      58.18
 H      -3.987403     0.684894    -5.036382      20.52
 C      -4.045201    -0.089361    -1.692782      33.19
 C      -4.041940    -1.299125    -0.771083      84.22
 H      -4.580535    -2.090062    -1.275871      27.42
 O      -4.765448    -1.052696     0.484493     133.26
 H      -4.102011    -0.496799     1.164108      21.97
 C      -2.659751    -1.986783    -0.544199      84.22
 H      -2.210238    -2.130789    -1.567944      26.45
 C      -2.792653    -3.343264     0.268066     115.55
 O      -3.361446    -4.263797    -0.737785     218.31
 H      -2.650649    -4.817262    -1.177641      27.83
 H      -3.549157    -3.198085     1.015261      26.78
 H      -1.878513    -3.793941     0.633779      26.32
 C       1.787935    -1.523921    -1.045307      53.62
 H       2.268897    -1.981423    -1.873270      22.61
 C       1.790234    -0.108484     0.932049      27.46
 H       2.453425     0.485585     1.670450      22.06
 C       0.331168    -0.192347     1.040161       1.05
 O      -0.434193     0.437878     2.032628     193.27
 C       0.324706     0.785317     3.253971     106.47
 H      -0.520493     0.796323     4.029766      25.08
 H       1.067365     0.032532     3.630852      26.99
 H       0.811488     1.796516     3.201585      24.89
 C      -0.352185    -1.067709     0.086541      -9.15
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 O      -1.787939    -1.026152     0.194511     131.34
 C       0.414874    -1.774216    -0.918183      72.11
 H      -0.162148    -2.232853    -1.677502      24.54
 C       2.522654    -0.677310    -0.161120      22.88
 C       4.034967    -0.432183    -0.387238      94.92
 H       4.279445    -0.559084    -1.474030      22.11
 O       4.286398     0.964369    -0.088577     252.67
 H       5.309912     1.050478    -0.083794      21.46
 C       4.929003    -1.570109     0.253728      92.74
 H       4.895380    -1.383542     1.320820      26.44
 O       4.373489    -2.868501    -0.036346     360.91
 H       4.649933    -3.213682    -0.986654      25.96
 C       6.427512    -1.495558    -0.247553      90.20
 O       6.996307    -0.172164     0.075259     315.40
 H       7.514124    -0.184195     0.882624      27.14
 H       6.277427    -1.621619    -1.366818      30.39
 H       7.000589    -2.380467     0.121996      30.13
55
name= lig-ACN-Water-frame_22
 C      -4.008350    -0.363063    -3.116393      29.92
 H      -4.003746    -1.399798    -3.509260      16.33
 C      -4.009766     1.217086    -1.170925      47.91
 H      -3.888376     1.395433    -0.082012      21.05
 C      -4.054583     2.354098    -2.082246      11.66
 O      -4.025841     3.678467    -1.607540     233.37
 C      -4.031260     3.994675    -0.183217     118.92
 H      -2.987223     3.958782     0.217022      28.65
 H      -4.681742     3.345022     0.355590      26.97
 H      -4.381890     5.004743    -0.151158      25.24
 C      -3.949186     2.166023    -3.442614      18.28
 O      -3.656924     3.084706    -4.397391     165.85
 H      -3.548006     4.070022    -3.975024      16.65
 C      -4.066311     0.818452    -3.950004      29.13
 H      -3.944066     0.638406    -5.053530      34.05
 C      -4.044462    -0.087594    -1.725436      38.06
 C      -4.071103    -1.297646    -0.773213      94.43
 H      -4.719464    -2.053778    -1.210069      28.12
 O      -4.727247    -1.066290     0.496615     142.65
 H      -4.103059    -0.540804     1.124981      24.90
 C      -2.628834    -2.014158    -0.536879      84.01
 H      -2.194890    -2.431948    -1.519907      27.41
 C      -2.880367    -3.308242     0.222800     117.95
 O      -3.428678    -4.301297    -0.711163     181.91
 H      -2.698480    -4.507223    -1.301465      30.49
 H      -3.535873    -3.253300     1.087954      27.21
 H      -1.922418    -3.544511     0.673161      28.08
 C       1.813020    -1.455482    -1.099923      45.29
 H       2.364611    -1.867649    -1.920890      20.91
 C       1.760895    -0.107114     0.930563      43.20
 H       2.154069     0.723380     1.612108      27.07
 C       0.378173    -0.219819     0.990065      -4.19
 O      -0.383081     0.423415     1.986364     200.01
 C       0.297092     0.764743     3.262940      99.38
 H      -0.466571     0.909077     4.101407      24.63
 H       0.990571    -0.087267     3.388476      26.40
 H       0.853933     1.762439     3.089893      22.63
 C      -0.353125    -1.029855     0.062890       3.11
 O      -1.781483    -1.054120     0.193130     143.48
 C       0.381442    -1.691191    -0.951334      69.51
 H      -0.037449    -2.422687    -1.649522      25.45
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 C       2.481889    -0.647362    -0.156805      25.43
 C       3.950657    -0.490176    -0.423789      93.86
 H       4.023846    -0.688807    -1.502439      21.51
 O       4.322607     0.916755    -0.127777     279.04
 H       5.308695     0.890055     0.068686      20.47
 C       4.969553    -1.575460     0.304686      95.16
 H       4.961587    -1.563963     1.365713      26.66
 O       4.364754    -2.803026    -0.015657     378.10
 H       4.702086    -3.086652    -0.938767      27.77
 C       6.394455    -1.462948    -0.259478     106.48
 O       7.000260    -0.158034     0.010008     328.74
 H       7.497576    -0.190664     0.852425      28.35
 H       6.498979    -1.490524    -1.385364      28.57
 H       7.083705    -2.258469     0.156191      27.83
55
name= lig-ACN-Water-frame_23
 C      -4.150783    -0.269165    -3.136522      54.45
 H      -4.033245    -1.285726    -3.604405      28.26
 C      -3.902364     1.226780    -1.194534      49.24
 H      -3.792595     1.395207    -0.060780      21.92
 C      -4.015981     2.321291    -2.016434      -2.28
 O      -4.020705     3.668925    -1.628786     221.70
 C      -4.057277     3.960248    -0.185584     119.72
 H      -3.056121     3.840816     0.223903      29.24
 H      -4.731672     3.359358     0.319462      28.04
 H      -4.376572     5.015298    -0.035116      25.50
 C      -3.887995     2.078416    -3.472466      -5.00
 O      -3.675839     3.134493    -4.387003      86.62
 H      -3.581106     4.118213    -3.961539      19.76
 C      -4.016065     0.803096    -4.023283      61.31
 H      -4.057735     0.767652    -5.112342      23.42
 C      -4.012265    -0.132541    -1.689901      -6.39
 C      -4.024197    -1.336191    -0.770111      87.51
 H      -4.600138    -2.126570    -1.276416      24.86
 O      -4.679341    -1.056602     0.518143     188.98
 H      -4.153312    -0.502158     1.031558      28.54
 C      -2.674575    -1.976172    -0.553841      85.74
 H      -2.172698    -1.996309    -1.599131      25.96
 C      -2.896429    -3.335892     0.216067     115.10
 O      -3.451511    -4.336216    -0.662469     200.82
 H      -2.893232    -4.451556    -1.472199      30.17
 H      -3.680257    -3.126035     0.970287      25.29
 H      -1.998452    -3.790467     0.587380      27.19
 C       1.722401    -1.393623    -1.117343      60.40
 H       2.246728    -1.892039    -1.940818      24.46
 C       1.741445    -0.030392     0.879716      47.80
 H       2.334940     0.593450     1.581641      22.93
 C       0.338367    -0.255853     0.998845       6.13
 O      -0.366177     0.395000     1.951751     218.34
 C       0.281880     0.719555     3.191384     113.58
 H      -0.594283     0.877768     3.882555      25.80
 H       0.940548    -0.016277     3.697573      26.40
 H       0.894404     1.704796     3.099368      26.21
 C      -0.391723    -1.027476     0.008522      17.16
 O      -1.729855    -1.098457     0.195483     173.20
 C       0.381630    -1.603503    -1.005391      79.29
 H      -0.136551    -2.390561    -1.618623      24.73
 C       2.445217    -0.678059    -0.162798       7.17
 C       3.964736    -0.507203    -0.412395     111.91
 H       4.188864    -0.656291    -1.461020      24.26
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 O       4.384564     0.859071    -0.140473     270.23
 H       5.328042     0.852641    -0.268655      24.71
 C       4.906003    -1.483241     0.288214      95.94
 H       4.955666    -1.252937     1.303658      27.14
 O       4.381906    -2.852201     0.029344     373.88
 H       4.447970    -3.026174    -0.934566      28.42
 C       6.398885    -1.410468    -0.269484      91.93
 O       7.024604    -0.096441    -0.030019     259.24
 H       7.630328    -0.178753     0.813388      23.71
 H       6.262547    -1.681942    -1.347267      31.00
 H       6.968115    -2.241871     0.251933      29.01
55
name= lig-ACN-Water-frame_24
 C      -4.212074    -0.245554    -3.096772      68.99
 H      -4.557497    -1.248706    -3.463132      35.08
 C      -3.842495     1.165895    -1.193594      53.71
 H      -3.876573     1.277448    -0.038713      23.26
 C      -3.882592     2.322173    -2.055122       7.89
 O      -4.016069     3.642141    -1.652931     200.89
 C      -4.076057     3.905000    -0.199555     120.89
 H      -3.174903     3.698186     0.296060      30.63
 H      -4.835448     3.354510     0.254324      28.39
 H      -4.256994     5.034710    -0.206111      26.50
 C      -3.856235     2.133963    -3.474232      19.56
 O      -3.726150     3.147109    -4.360280     112.67
 H      -3.502837     4.062417    -3.914383      24.03
 C      -3.974380     0.813993    -4.019808      37.27
 H      -4.024871     0.577026    -5.050957      16.29
 C      -3.997893    -0.088608    -1.745352       6.35
 C      -4.002570    -1.300438    -0.748057      77.95
 H      -4.622819    -2.126581    -1.153445      26.52
 O      -4.642180    -1.032349     0.522182     174.95
 H      -4.026192    -0.597436     1.130165      26.98
 C      -2.589376    -1.981594    -0.587497      86.65
 H      -2.259810    -2.335343    -1.646591      26.72
 C      -2.837006    -3.367437     0.172841     104.82
 O      -3.487589    -4.378634    -0.663041     196.30
 H      -2.768372    -4.635339    -1.349475      28.56
 H      -3.532277    -3.196937     1.037675      25.82
 H      -1.922748    -3.633722     0.696877      27.28
 C       1.708499    -1.396001    -1.169891      50.13
 H       2.236512    -1.894814    -2.029398      24.99
 C       1.740272    -0.026447     0.810074      64.28
 H       2.212042     0.463626     1.623403      26.96
 C       0.365786    -0.241848     0.945726      17.07
 O      -0.425709     0.349788     1.959198     194.43
 C       0.237476     0.727165     3.196936     113.05
 H      -0.560925     1.039798     3.903917      26.20
 H       0.775978    -0.186987     3.505082      26.12
 H       0.897199     1.655144     3.055900      25.66
 C      -0.377087    -1.006526     0.018089      13.94
 O      -1.778074    -1.124324     0.247469     157.65
 C       0.264940    -1.607189    -1.088050      65.70
 H      -0.253118    -2.080662    -1.984143      21.50
 C       2.486115    -0.645782    -0.218534       6.58
 C       3.964118    -0.481710    -0.478076     128.53
 H       4.005314    -0.669399    -1.526255      22.24
 O       4.436069     0.864397    -0.135819     276.34
 H       5.380921     0.954030    -0.427203      19.86
 C       4.862070    -1.488447     0.270095     106.20
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 H       4.726581    -1.368428     1.289626      27.12
 O       4.434566    -2.867454     0.123853     358.28
 H       4.690821    -3.176840    -0.767969      30.04
 C       6.332643    -1.381057    -0.220586      98.24
 O       7.061620    -0.055709    -0.092789     278.00
 H       7.605836    -0.055785     0.843707      24.20
 H       6.467727    -1.485843    -1.300923      29.39
 H       6.945006    -2.197103     0.260693      27.78
55
name= lig-ACN-Water-frame_25
 C      -4.214491    -0.294267    -3.109827      62.63
 H      -4.580651    -1.223459    -3.552181      29.87
 C      -3.802891     1.241305    -1.201502      52.18
 H      -3.802249     1.415105    -0.087425      23.76
 C      -3.761799     2.294199    -2.076509      13.63
 O      -3.969889     3.607116    -1.649258     199.16
 C      -4.098812     3.865444    -0.249430     121.29
 H      -3.260579     3.526838     0.232527      31.09
 H      -5.037706     3.478889     0.121823      27.30
 H      -4.159861     5.000413    -0.072143      26.33
 C      -3.788743     2.117236    -3.456821      10.69
 O      -3.781062     3.184892    -4.388412     100.19
 H      -3.659720     4.129557    -4.022075      22.34
 C      -3.992065     0.827788    -3.949913      43.17
 H      -4.045674     0.783265    -5.003116      22.34
 C      -4.014539    -0.120427    -1.690629     -56.76
 C      -3.995622    -1.289129    -0.783608      61.77
 H      -4.709130    -2.001608    -1.260368      23.97
 O      -4.590599    -0.980636     0.545810     124.30
 H      -3.858835    -0.595586     1.244464      23.60
 C      -2.609949    -2.075093    -0.579803      92.53
 H      -1.967735    -2.113773    -1.507757      25.81
 C      -2.770094    -3.374931     0.165036     113.98
 O      -3.424050    -4.393779    -0.673096     216.92
 H      -2.766986    -4.908555    -1.160035      30.63
 H      -3.421920    -3.240586     1.070855      25.16
 H      -1.795759    -3.821405     0.335593      26.37
 C       1.677779    -1.422278    -1.240446      53.39
 H       2.212651    -1.780979    -2.167637      18.23
 C       1.762388    -0.056052     0.811634      46.39
 H       2.283993     0.590346     1.435758      28.05
 C       0.323518    -0.198410     0.919092      -6.06
 O      -0.481959     0.311489     1.953930     171.13
 C       0.197553     0.721205     3.207522     120.35
 H      -0.539876     1.047835     3.933231      26.84
 H       0.768249    -0.104136     3.697473      27.66
 H       0.971882     1.480956     2.963087      25.38
 C      -0.438265    -1.035139    -0.023824       8.68
 O      -1.779414    -1.139543     0.275600     146.49
 C       0.291889    -1.534994    -1.136812      74.93
 H      -0.271904    -2.028762    -1.965330      26.35
 C       2.404888    -0.626338    -0.353511      34.57
 C       3.941575    -0.465915    -0.588346      77.36
 H       4.248670    -0.522668    -1.597018      24.99
 O       4.429468     0.908408    -0.149950     239.04
 H       5.441582     0.825342    -0.330210      21.50
 C       4.855602    -1.513958     0.299515      76.66
 H       4.816813    -1.169329     1.290871      26.81
 O       4.509504    -2.895926     0.182978     337.23
 H       4.881306    -3.234802    -0.686948      27.50
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 C       6.355263    -1.338538    -0.188338     104.90
 O       7.053079    -0.054063    -0.118400     254.30
 H       7.652382    -0.132961     0.767812      23.18
 H       6.244823    -1.676736    -1.202667      31.86
 H       6.964207    -2.058969     0.393594      28.94
55
name= lig-ACN-Water-frame_26
 C      -4.155873    -0.271172    -3.068983      80.89
 H      -4.090812    -1.262787    -3.469393      27.65
 C      -3.770917     1.192023    -1.192417      67.60
 H      -3.718235     1.369238    -0.140890      22.18
 C      -3.727105     2.349266    -2.035169      -4.56
 O      -3.877692     3.638768    -1.677441     170.04
 C      -4.120930     3.842581    -0.246380     117.27
 H      -3.465454     3.392036     0.385818      29.95
 H      -5.099765     3.410830     0.083609      25.69
 H      -4.025491     4.960029    -0.180445      25.36
 C      -3.732787     2.139647    -3.503203      -2.09
 O      -3.832858     3.169812    -4.433128     126.06
 H      -3.708323     4.058274    -4.037125      21.89
 C      -4.033232     0.819526    -3.957201      22.24
 H      -4.258053     0.681461    -5.008180      22.73
 C      -3.986726    -0.087074    -1.696125      18.30
 C      -4.005327    -1.350713    -0.736832      82.55
 H      -4.654633    -2.180240    -1.122793      25.84
 O      -4.541613    -0.957924     0.553935     157.16
 H      -3.798678    -0.396063     1.049114      23.51
 C      -2.648196    -2.013872    -0.577109      91.85
 H      -2.371397    -2.252407    -1.634892      27.49
 C      -2.670592    -3.475165     0.135724     109.08
 O      -3.367513    -4.414360    -0.676273     236.35
 H      -2.663156    -4.758884    -1.259058      29.78
 H      -3.155116    -3.376072     1.142496      26.17
 H      -1.626344    -3.700715     0.436364      26.80
 C       1.662770    -1.369188    -1.357689      55.61
 H       2.075894    -1.877204    -2.264213      16.46
 C       1.696419    -0.077246     0.722386      58.43
 H       2.281774     0.540691     1.350866      26.75
 C       0.295516    -0.224591     0.915556      23.28
 O      -0.468335     0.279808     1.972425     197.37
 C       0.195830     0.706322     3.187265     122.38
 H      -0.635318     1.155042     3.696121      26.13
 H       0.614159    -0.177936     3.703270      27.07
 H       0.846595     1.545517     3.025814      26.03
 C      -0.407282    -0.983607    -0.031731       6.04
 O      -1.781396    -1.185411     0.268615     143.44
 C       0.251076    -1.514146    -1.168113      71.56
 H      -0.223525    -2.249415    -1.797260      24.45
 C       2.407244    -0.587404    -0.416761      19.71
 C       3.958047    -0.458959    -0.575215     108.78
 H       4.101587    -0.682755    -1.605808      23.06
 O       4.365588     0.897526    -0.190129     277.31
 H       5.352902     0.916055    -0.163689      22.50
 C       4.866862    -1.406293     0.279225      88.90
 H       4.637066    -1.230784     1.313973      25.02
 O       4.599961    -2.912805     0.225841     350.62
 H       4.771832    -3.156339    -0.760517      25.72
 C       6.380269    -1.410110    -0.175553     110.86
 O       7.010931    -0.050223    -0.132942     281.41
 H       7.662648    -0.028535     0.667206      26.15
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 H       6.574964    -1.701866    -1.182190      29.41
 H       6.919252    -2.108171     0.450398      28.83
55
name= lig-ACN-Water-frame_27
 C      -4.019253    -0.279069    -3.074081      45.39
 H      -4.152313    -1.259569    -3.486545      18.50
 C      -3.748564     1.214131    -1.169359      39.41
 H      -3.744475     1.345230    -0.147241      19.93
 C      -3.732260     2.300613    -2.118482       0.73
 O      -3.752418     3.698031    -1.646589     193.15
 C      -4.133094     3.867048    -0.227316     111.11
 H      -3.424845     3.406613     0.355893      27.64
 H      -5.234477     3.534542    -0.140230      24.10
 H      -4.155383     4.930181     0.012486      24.07
 C      -3.802569     2.127339    -3.503225      16.35
 O      -3.866571     3.133075    -4.467502     188.13
 H      -3.769097     4.032854    -4.117660      22.13
 C      -4.049900     0.831272    -3.991094      46.00
 H      -4.179111     0.603179    -5.079282      30.00
 C      -3.925880    -0.138942    -1.672076      14.00
 C      -4.010838    -1.318554    -0.672102     101.77
 H      -4.749003    -2.053753    -1.096947      25.65
 O      -4.530228    -0.949986     0.580248     202.16
 H      -3.964272    -0.395854     1.062231      26.66
 C      -2.619413    -2.080099    -0.562731      93.66
 H      -2.156757    -2.110738    -1.538645      25.37
 C      -2.589673    -3.436981     0.132820     115.98
 O      -3.280807    -4.480864    -0.692831     203.79
 H      -2.818575    -4.543920    -1.602291      29.00
 H      -3.153984    -3.491598     1.077728      25.22
 H      -1.539211    -3.800092     0.183894      24.36
 C       1.622492    -1.280183    -1.418308      50.24
 H       2.185552    -1.789585    -2.198841      24.88
 C       1.683591    -0.034961     0.632741      59.16
 H       2.161600     0.426004     1.509052      23.82
 C       0.320548    -0.262664     0.897827      11.16
 O      -0.412773     0.243232     1.950428     205.78
 C       0.161680     0.740104     3.189546     124.34
 H      -0.591849     1.106134     3.856873      26.07
 H       0.640703    -0.108578     3.717517      26.67
 H       0.967597     1.375498     2.995722      26.69
 C      -0.453775    -0.989420    -0.086746      15.29
 O      -1.759184    -1.206674     0.214200     188.44
 C       0.231816    -1.571166    -1.173043      78.85
 H      -0.335708    -2.155507    -1.835782      22.15
 C       2.403810    -0.615656    -0.451794      25.89
 C       3.923927    -0.490092    -0.567014      96.55
 H       4.231661    -0.595716    -1.596298      20.00
 O       4.284844     0.892698    -0.247587     277.23
 H       5.234155     0.838926    -0.259294      21.53
 C       4.904859    -1.472654     0.246444      92.13
 H       4.930434    -1.082042     1.288905      20.94
 O       4.642566    -2.849259     0.216806     348.18
 H       4.802767    -3.182234    -0.723879      26.56
 C       6.398152    -1.417167    -0.148855     108.14
 O       6.972911    -0.031043    -0.140570     314.69
 H       7.385365    -0.058974     0.790039      27.28
 H       6.430682    -1.860254    -1.117485      31.71
 H       6.912558    -1.987969     0.583975      28.99
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name= lig-ACN-Water-frame_28
 C      -3.934185    -0.331247    -3.099023      57.36
 H      -4.209639    -1.293117    -3.513397      23.85
 C      -3.756049     1.235390    -1.235111      47.22
 H      -3.707627     1.492082    -0.220786      17.10
 C      -3.755269     2.366223    -2.055855      16.99
 O      -3.616765     3.663562    -1.626824     225.24
 C      -4.144688     3.908470    -0.255487      92.74
 H      -3.565528     3.442119     0.534749      29.13
 H      -5.163073     3.364904    -0.060462      26.76
 H      -4.110150     4.949614    -0.140110      25.99
 C      -3.941299     2.107864    -3.524605      -3.48
 O      -3.889189     3.126487    -4.490211      57.48
 H      -3.911516     4.019152    -4.018012      24.35
 C      -3.981235     0.753350    -3.966071      53.76
 H      -4.045665     0.702619    -5.107464      17.22
 C      -3.833221    -0.095209    -1.667832      21.57
 C      -3.953802    -1.307467    -0.703804      69.30
 H      -4.724300    -1.999720    -1.121276      23.25
 O      -4.566187    -0.944007     0.660685     192.46
 H      -3.888216    -0.514203     1.179317      25.17
 C      -2.580538    -2.093070    -0.592607      93.11
 H      -2.276377    -2.258220    -1.594984      24.56
 C      -2.566835    -3.505800     0.063922     114.81
 O      -3.222034    -4.514110    -0.708657     303.90
 H      -2.674961    -4.514318    -1.552379      28.76
 H      -2.968220    -3.366393     1.071579      25.13
 H      -1.483314    -3.724312     0.289229      24.37
 C       1.601354    -1.308256    -1.418608      30.60
 H       1.986768    -1.629732    -2.358783      24.41
 C       1.718623    -0.023790     0.671690      40.45
 H       2.460223     0.531706     1.337383      20.96
 C       0.333383    -0.270235     0.822483      12.30
 O      -0.407351     0.212408     1.934796     186.15
 C       0.234359     0.715514     3.183438     118.23
 H      -0.640415     1.210695     3.588933      25.20
 H       0.644418    -0.078831     3.805739      26.25
 H       0.836208     1.545113     3.013585      27.18
 C      -0.426652    -1.052864    -0.119631      16.58
 O      -1.776274    -1.179186     0.215486     183.83
 C       0.253679    -1.587230    -1.236026      66.45
 H      -0.195305    -2.079639    -2.058027      16.73
 C       2.369317    -0.628337    -0.447125      27.28
 C       3.914832    -0.531016    -0.636594      94.37
 H       4.087767    -0.785858    -1.690443      19.65
 O       4.223846     0.907054    -0.288689     247.87
 H       5.215230     1.038242    -0.333481      20.03
 C       4.944885    -1.451362     0.280987      85.01
 H       4.740191    -1.216532     1.379112      21.93
 O       4.602856    -2.859354     0.189130     364.01
 H       4.893826    -3.116103    -0.708540      28.09
 C       6.415810    -1.364969    -0.166211     123.57
 O       6.910919    -0.018454    -0.144267     331.67
 H       7.519916     0.054915     0.629623      28.40
 H       6.698340    -1.753711    -1.135386      30.58
 H       6.976326    -1.983003     0.495041      28.18
55
name= lig-ACN-Water-frame_29
 C      -3.915450    -0.370931    -3.057044      63.88
 H      -3.750949    -1.420054    -3.371925      23.99
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 C      -3.751860     1.256935    -1.232342      42.42
 H      -3.629905     1.289236    -0.137614      20.75
 C      -3.811420     2.358902    -2.141644      15.84
 O      -3.520264     3.627362    -1.581157     276.58
 C      -4.120019     3.935898    -0.290539      97.03
 H      -3.410652     3.650494     0.533308      27.82
 H      -5.209355     3.551148    -0.287364      25.80
 H      -4.260063     4.973594    -0.304874      26.72
 C      -3.969274     2.130156    -3.475217      19.71
 O      -3.933850     3.102306    -4.461848     149.80
 H      -3.875722     4.092948    -4.084400      23.14
 C      -3.905988     0.757575    -3.962440      37.08
 H      -4.036407     0.441728    -5.051630      18.94
 C      -3.795200    -0.081880    -1.718940      14.22
 C      -3.939315    -1.300608    -0.666662      80.80
 H      -4.655024    -2.024568    -1.107569      25.37
 O      -4.539599    -0.971580     0.631170     186.09
 H      -3.879966    -0.448767     1.309932      21.26
 C      -2.613340    -2.057345    -0.630606      94.56
 H      -2.224144    -2.067556    -1.596684      24.96
 C      -2.542355    -3.508294     0.080083     110.96
 O      -3.187455    -4.523889    -0.737566     277.24
 H      -2.551283    -4.944923    -1.305038      31.03
 H      -3.151465    -3.592769     0.967270      24.81
 H      -1.474375    -3.803004     0.221384      25.31
 C       1.660640    -1.372546    -1.420040      40.32
 H       2.222569    -1.659388    -2.282499      16.84
 C       1.758351    -0.103779     0.672436      51.57
 H       2.137177     0.655217     1.454497      24.86
 C       0.370078    -0.249328     0.846176       8.62
 O      -0.388057     0.170616     1.917658     208.24
 C       0.235904     0.735836     3.094637     129.05
 H      -0.536717     1.081399     3.791583      25.52
 H       0.725260    -0.072164     3.633943      27.10
 H       1.026314     1.388135     2.878363      24.48
 C      -0.366657    -1.082027    -0.084887       1.14
 O      -1.748237    -1.173698     0.187966     147.89
 C       0.215564    -1.559057    -1.310370      74.43
 H      -0.399023    -2.130821    -2.021534      22.00
 C       2.425191    -0.662767    -0.448824      39.41
 C       3.919212    -0.517466    -0.636031      96.58
 H       4.215670    -0.686722    -1.706758      20.17
 O       4.177589     0.908622    -0.348058     246.28
 H       5.186827     0.991315    -0.519916      20.13
 C       4.858228    -1.436552     0.227703      65.84
 H       4.783004    -1.101422     1.346349      22.10
 O       4.548910    -2.894599     0.158013     344.11
 H       4.592541    -3.115337    -0.811638      27.28
 C       6.424942    -1.338798    -0.178140      90.33
 O       6.891269     0.076945    -0.154666     359.80
 H       7.455769     0.021923     0.625405      27.14
 H       6.332704    -1.672584    -1.208125      30.61
 H       7.021378    -1.954308     0.475153      27.11
55
name= lig-ACN-Water-frame_30
 C      -3.833765    -0.313772    -3.062493      51.51
 H      -3.765234    -1.320608    -3.557700      21.62
 C      -3.753121     1.197570    -1.215394      53.64
 H      -3.670009     1.607614    -0.149751      18.82
 C      -3.795852     2.307442    -2.044755       5.66
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 O      -3.462585     3.599905    -1.607676     239.04
 C      -4.120580     4.021817    -0.361263     105.22
 H      -3.499977     3.660787     0.575473      25.72
 H      -5.033083     3.404935    -0.136407      24.37
 H      -4.192130     5.086094    -0.320566      25.30
 C      -3.900886     2.067257    -3.531187       5.67
 O      -3.995142     3.107740    -4.446947      78.07
 H      -3.842921     4.006715    -3.906593      22.34
 C      -3.907139     0.739402    -3.948480      64.97
 H      -3.872051     0.700696    -5.059033      24.53
 C      -3.863249    -0.127006    -1.604736      23.83
 C      -3.949295    -1.276954    -0.679528     104.45
 H      -4.698927    -1.949608    -1.128394      26.66
 O      -4.494019    -1.001771     0.570914     194.60
 H      -3.901171    -0.345399     1.201904      22.11
 C      -2.565404    -2.061019    -0.572370     103.91
 H      -2.289415    -2.227393    -1.577039      28.43
 C      -2.588312    -3.462607     0.054778     117.41
 O      -3.192108    -4.546863    -0.760661     248.99
 H      -2.400108    -4.833751    -1.316006      28.64
 H      -3.032554    -3.320496     1.024593      26.99
 H      -1.530706    -3.687648     0.299761      26.67
 C       1.692026    -1.423238    -1.417503      53.49
 H       2.125019    -2.004723    -2.228778      25.62
 C       1.759150    -0.150123     0.684831      -9.81
 H       2.508153     0.373052     1.354630      22.64
 C       0.382618    -0.355277     0.853599       4.76
 O      -0.413202     0.171234     1.899991     192.46
 C       0.309082     0.695474     3.033796     125.82
 H      -0.457343     1.193691     3.657616      27.33
 H       0.861439    -0.081857     3.520860      27.87
 H       0.868712     1.567237     2.730175      28.68
 C      -0.369026    -1.073277    -0.129137      22.04
 O      -1.677204    -1.171203     0.171248     171.50
 C       0.299720    -1.513570    -1.246495      76.90
 H      -0.251270    -2.077209    -2.067845      25.18
 C       2.432233    -0.742143    -0.452080     -31.74
 C       3.928715    -0.489595    -0.648406     123.45
 H       4.149652    -0.700218    -1.751879      20.59
 O       4.189552     0.909542    -0.385370     261.46
 H       5.095927     1.084520    -0.630457      23.29
 C       4.842108    -1.478751     0.199911      74.89
 H       4.652983    -1.192360     1.329498      23.42
 O       4.470809    -2.844419     0.143430     347.01
 H       4.618252    -3.170931    -0.811175      27.20
 C       6.275331    -1.268845    -0.244090     105.57
 O       6.883915     0.135896    -0.152563     293.06
 H       7.543256     0.159536     0.528867      25.76
 H       6.571997    -1.565688    -1.264130      27.96
 H       6.931975    -1.931449     0.354497      27.25
55
name= lig-ACN-Water-frame_31
 C      -3.798302    -0.313271    -3.017959      32.57
 H      -4.005148    -1.372876    -3.323563      19.12
 C      -3.782994     1.205538    -1.112541      42.72
 H      -3.770511     1.243458     0.039373      20.78
 C      -3.696432     2.271265    -2.084788      21.52
 O      -3.474331     3.578281    -1.663514     245.23
 C      -4.095703     4.040461    -0.387435      96.13
 H      -3.331564     3.843554     0.511604      25.69
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 H      -5.113411     3.701516    -0.327613      25.83
 H      -4.215515     5.138340    -0.591188      24.48
 C      -3.829077     2.111058    -3.447699      23.73
 O      -4.036770     3.096917    -4.390897     203.58
 H      -3.977660     4.079858    -4.084657      19.50
 C      -3.875143     0.773419    -3.975787      45.79
 H      -3.883010     0.459371    -4.997969      30.36
 C      -3.902932    -0.105580    -1.669792      24.34
 C      -3.906721    -1.381137    -0.733390     100.83
 H      -4.526640    -2.196462    -1.138359      28.73
 O      -4.514132    -1.015071     0.589907     123.84
 H      -3.932224    -0.443718     1.096629      26.40
 C      -2.555354    -2.058600    -0.641120      95.25
 H      -2.100065    -2.158716    -1.615712      27.76
 C      -2.632761    -3.439842     0.110036     115.25
 O      -3.186464    -4.500438    -0.727725     204.65
 H      -2.661565    -4.538909    -1.612375      28.76
 H      -3.291033    -3.520889     0.955816      26.65
 H      -1.610427    -3.743073     0.353293      26.61
 C       1.726706    -1.488368    -1.394569      50.66
 H       2.206956    -1.908367    -2.314299      24.79
 C       1.800446    -0.243049     0.677876      65.24
 H       2.308453     0.251118     1.494322      30.14
 C       0.397618    -0.410635     0.892310      -1.68
 O      -0.410042     0.151229     1.862211     176.64
 C       0.367506     0.730286     2.990515     112.68
 H      -0.407953     0.948529     3.743357      27.38
 H       1.035260     0.030934     3.470734      26.23
 H       1.033087     1.544079     2.645287      27.59
 C      -0.317609    -1.018665    -0.137483       4.58
 O      -1.701590    -1.188411     0.162745     158.02
 C       0.337190    -1.585983    -1.263051      75.58
 H      -0.264635    -2.084790    -2.100489      23.73
 C       2.453056    -0.762443    -0.445084      34.01
 C       3.884992    -0.544185    -0.688054     116.45
 H       4.119170    -0.773197    -1.803008      24.05
 O       4.214798     0.931081    -0.390980     247.39
 H       5.159809     1.034854    -0.605129      22.14
 C       4.805424    -1.382249     0.183080      80.47
 H       4.794843    -1.092072     1.320858      24.48
 O       4.397131    -2.798975     0.130733     316.13
 H       4.690656    -3.151879    -0.798480      27.80
 C       6.313886    -1.205473    -0.293107      87.39
 O       6.832609     0.142429    -0.153330     254.01
 H       7.527432     0.022692     0.511139      23.54
 H       6.219608    -1.510198    -1.362158      29.01
 H       6.914724    -1.908167     0.355289      27.49
55
name= lig-ACN-Water-frame_32
 C      -3.891060    -0.324360    -3.064021      61.54
 H      -3.814776    -1.312054    -3.547080      24.78
 C      -3.812595     1.186229    -1.124085      59.93
 H      -3.870896     1.489513    -0.043469      17.47
 C      -3.601792     2.262367    -1.974996      10.82
 O      -3.510985     3.604564    -1.697574     270.96
 C      -4.066156     4.090725    -0.506017     102.15
 H      -3.444913     3.709766     0.475896      27.53
 H      -4.985612     3.657692    -0.260596      29.33
 H      -3.999600     5.251400    -0.515503      23.91
 C      -3.788818     2.056439    -3.458354      -5.89
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 O      -4.054202     3.114486    -4.344005     152.58
 H      -3.958159     3.952540    -3.857338      23.95
 C      -3.791821     0.751719    -3.932731      66.07
 H      -4.070765     0.719718    -4.934507      23.87
 C      -3.876895    -0.135614    -1.635631      33.47
 C      -3.945155    -1.375605    -0.765396      85.13
 H      -4.669139    -2.065549    -1.207929      25.13
 O      -4.536913    -1.092072     0.544525     170.84
 H      -3.944953    -0.645148     1.088545      27.03
 C      -2.517404    -2.080150    -0.636398      93.99
 H      -2.197033    -2.263849    -1.693055      24.58
 C      -2.644725    -3.463328     0.136139     117.53
 O      -3.230675    -4.446316    -0.717728     258.76
 H      -2.666870    -4.462518    -1.519119      30.50
 H      -3.323726    -3.179847     0.940824      26.27
 H      -1.714093    -3.715331     0.630112      27.02
 C       1.731931    -1.513224    -1.408818      50.76
 H       2.312399    -1.760043    -2.345052      14.47
 C       1.806760    -0.312709     0.778864      61.11
 H       2.393160     0.263807     1.405383      24.33
 C       0.421452    -0.397436     0.843947       5.09
 O      -0.317005     0.143904     1.903373     189.23
 C       0.396672     0.740422     2.966241     124.23
 H      -0.261070     1.098686     3.771302      25.61
 H       1.109435    -0.008494     3.284504      26.09
 H       0.866593     1.727647     2.642072      24.18
 C      -0.373114    -1.116994    -0.176963      14.28
 O      -1.690647    -1.172008     0.136432     181.25
 C       0.292431    -1.677452    -1.277489      67.29
 H      -0.287556    -2.232561    -2.043539      21.25
 C       2.433510    -0.779667    -0.442045      21.16
 C       3.917588    -0.473295    -0.687997      86.21
 H       4.170385    -0.673681    -1.812779      22.22
 O       4.205434     0.914947    -0.421711     265.10
 H       5.245618     0.975854    -0.439149      18.60
 C       4.847243    -1.337847     0.186921      85.22
 H       4.651268    -0.897082     1.241509      24.02
 O       4.398258    -2.712211     0.145196     336.26
 H       4.481089    -2.999838    -0.857572      28.04
 C       6.291798    -1.248333    -0.320115     103.31
 O       6.815927     0.128985    -0.149928     254.63
 H       7.464925     0.174204     0.661499      25.16
 H       6.430106    -1.410964    -1.420871      29.57
 H       7.044912    -2.002270     0.095010      28.68
55
name= lig-ACN-Water-frame_33
 C      -3.924610    -0.363850    -3.054739      57.64
 H      -4.021666    -1.392615    -3.404349      25.86
 C      -3.785916     1.180854    -1.138339      60.24
 H      -3.895626     1.283348    -0.074230      19.15
 C      -3.614414     2.272296    -2.055456      16.77
 O      -3.514573     3.648835    -1.767170     259.25
 C      -4.050069     4.112910    -0.478549      97.22
 H      -3.360169     3.670383     0.396349      27.74
 H      -5.063766     3.920195    -0.445120      29.76
 H      -3.986810     5.279280    -0.568317      24.68
 C      -3.730449     2.063628    -3.403151      17.08
 O      -4.027393     3.082158    -4.252544     173.27
 H      -3.982733     3.983080    -3.935300      25.60
 C      -3.804044     0.767725    -3.956087      64.19
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 H      -3.876055     0.595733    -4.984512      26.06
 C      -3.860988    -0.153458    -1.666088      14.99
 C      -3.975902    -1.376647    -0.760443      83.79
 H      -4.579040    -2.117262    -1.288337      25.45
 O      -4.555719    -1.176888     0.498029     171.40
 H      -3.955476    -0.645634     1.095342      22.42
 C      -2.570960    -2.119540    -0.606015      96.25
 H      -2.111201    -2.298808    -1.634784      23.67
 C      -2.679852    -3.377843     0.180245     117.55
 O      -3.289335    -4.415345    -0.713665     226.27
 H      -2.581333    -4.792713    -1.244409      29.75
 H      -3.376156    -3.348925     1.042694      25.44
 H      -1.748994    -3.785872     0.506589      26.66
 C       1.655680    -1.460418    -1.415909      39.87
 H       2.074054    -1.933972    -2.338848      21.43
 C       1.830549    -0.348652     0.748325      44.57
 H       2.373286     0.170942     1.458664      24.66
 C       0.402362    -0.411556     0.813205       7.43
 O      -0.288501     0.119999     1.912000     176.74
 C       0.487228     0.782004     2.981623     116.27
 H      -0.326765     0.888799     3.687917      24.98
 H       1.305749     0.275756     3.515201      25.68
 H       0.952053     1.757381     2.586360      23.76
 C      -0.323461    -1.190424    -0.129480       5.33
 O      -1.714174    -1.166181     0.074656     169.99
 C       0.318163    -1.757530    -1.271696      57.93
 H      -0.144990    -2.325741    -2.028856      19.83
 C       2.448053    -0.786333    -0.433783      27.43
 C       3.923426    -0.426958    -0.697823      85.49
 H       4.104241    -0.682897    -1.827056      21.08
 O       4.194622     0.967815    -0.446073     270.88
 H       5.175789     1.050995    -0.242688      21.11
 C       4.886244    -1.332938     0.167765      81.75
 H       4.980105    -1.092953     1.277322      22.82
 O       4.424917    -2.656057     0.165787     301.99
 H       4.556226    -2.994009    -0.802065      26.97
 C       6.333045    -1.277564    -0.358213      89.67
 O       6.836334     0.113571    -0.122200     262.11
 H       7.522325    -0.010369     0.704711      23.71
 H       6.259192    -1.500300    -1.447611      29.46
 H       6.892244    -2.040635     0.273977      27.32
55
name= lig-ACN-Water-frame_34
 C      -3.904657    -0.355504    -3.064645      48.90
 H      -4.183445    -1.310874    -3.483334      19.81
 C      -3.710778     1.188124    -1.158111      55.90
 H      -3.700134     1.346836    -0.135570      21.05
 C      -3.669349     2.291690    -2.022931      17.77
 O      -3.516596     3.656137    -1.783091     216.51
 C      -4.029905     4.135466    -0.491986     107.98
 H      -3.545449     3.619710     0.451362      26.26
 H      -5.051002     3.892147    -0.334289      24.94
 H      -3.735836     5.222615    -0.487463      24.34
 C      -3.726635     2.012536    -3.442294       5.84
 O      -3.979499     3.098315    -4.276136     140.42
 H      -3.918180     3.891306    -3.665111      23.82
 C      -3.841515     0.693915    -3.957961      60.28
 H      -3.826111     0.569530    -5.032376      24.30
 C      -3.894223    -0.128830    -1.701553      38.44
 C      -3.937734    -1.434722    -0.822567      90.64
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 H      -4.594414    -2.166868    -1.284392      27.50
 O      -4.602009    -1.207396     0.503640      67.49
 H      -4.015879    -0.537939     1.134209      21.89
 C      -2.619256    -2.069192    -0.620499      92.75
 H      -2.272807    -2.442607    -1.659479      28.40
 C      -2.736304    -3.451654     0.202934     118.97
 O      -3.348274    -4.386301    -0.673137     211.25
 H      -2.605199    -4.875593    -1.167076      27.36
 H      -3.318387    -3.320421     1.150688      27.06
 H      -1.702263    -3.607227     0.432595      27.24
 C       1.717095    -1.444690    -1.442549      48.30
 H       2.289664    -1.780858    -2.316552      26.15
 C       1.802301    -0.327394     0.663112      71.35
 H       2.345035     0.088096     1.496312      25.12
 C       0.443930    -0.481727     0.876796      11.92
 O      -0.245935     0.080857     1.928607     185.39
 C       0.507766     0.834233     2.998059     104.63
 H      -0.137982     1.131710     3.817433      26.23
 H       1.292153     0.089603     3.265118      24.35
 H       0.920255     1.828065     2.581163      26.22
 C      -0.355950    -1.219546    -0.093784      12.63
 O      -1.716044    -1.149201     0.050483     156.33
 C       0.311317    -1.772807    -1.182694      77.53
 H      -0.267538    -2.259430    -1.891205      23.75
 C       2.465974    -0.766137    -0.495062      40.28
 C       3.918921    -0.469961    -0.682324      90.87
 H       4.221268    -0.641271    -1.782981      21.83
 O       4.184103     1.043721    -0.448825     248.14
 H       5.127715     1.071930    -0.318563      23.80
 C       4.922332    -1.295931     0.144797      89.10
 H       4.842011    -0.835131     1.155594      25.00
 O       4.446203    -2.715350     0.158866     306.61
 H       4.613985    -3.035529    -0.757915      29.51
 C       6.371900    -1.263362    -0.358801     106.26
 O       6.889033     0.057476    -0.098672     281.70
 H       7.738174     0.056301     0.563127      23.26
 H       6.554564    -1.505693    -1.433228      28.95
 H       7.036977    -1.999976     0.159374      27.82
55
name= lig-ACN-Water-frame_35
 C      -3.942330    -0.389397    -3.102944      45.20
 H      -3.916212    -1.428382    -3.459559      25.12
 C      -3.656111     1.188437    -1.149384      50.54
 H      -3.518669     1.410501    -0.137469      21.41
 C      -3.684428     2.252988    -2.074677      13.19
 O      -3.533244     3.611087    -1.737778     252.58
 C      -3.987523     4.118038    -0.482211     103.39
 H      -3.452343     3.517467     0.307897      28.72
 H      -5.093567     4.080705    -0.437114      25.51
 H      -3.698977     5.121560    -0.458461      26.60
 C      -3.813988     2.012949    -3.491512      13.74
 O      -3.891450     3.096071    -4.340091     113.09
 H      -3.978417     4.045254    -3.883148      23.07
 C      -3.832005     0.718768    -4.002453      60.70
 H      -4.122144     0.578679    -5.086279      22.34
 C      -3.901368    -0.157437    -1.650089      13.88
 C      -4.008834    -1.362545    -0.798866      90.68
 H      -4.615654    -2.079121    -1.355584      25.16
 O      -4.641553    -1.191695     0.457587     165.99
 H      -4.073818    -0.509534     1.086151      21.51
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 C      -2.593133    -2.138308    -0.613222      91.24
 H      -2.132722    -2.265269    -1.658280      25.77
 C      -2.705127    -3.415446     0.178360     113.13
 O      -3.416479    -4.424205    -0.619418     194.60
 H      -2.784292    -4.660305    -1.361878      28.55
 H      -3.374447    -3.269935     1.069041      26.21
 H      -1.816126    -3.935022     0.536512      25.91
 C       1.725795    -1.513702    -1.472004      44.29
 H       2.049780    -1.837321    -2.444075      20.49
 C       1.819085    -0.281903     0.672978      38.87
 H       2.516994     0.360414     1.304870      20.74
 C       0.433073    -0.541496     0.945359      11.61
 O      -0.238766     0.077155     2.003439     192.06
 C       0.522593     0.812960     2.933138     116.72
 H      -0.233796     1.027148     3.698579      25.73
 H       1.378412     0.281678     3.493487      25.63
 H       1.023555     1.714203     2.446680      26.43
 C      -0.322745    -1.195484    -0.049853       6.93
 O      -1.752542    -1.128516     0.070424     144.98
 C       0.378959    -1.730563    -1.182633      65.47
 H      -0.159970    -2.237704    -1.959509      23.24
 C       2.467072    -0.717653    -0.531344      17.28
 C       3.977890    -0.399914    -0.758082      94.85
 H       4.147712    -0.591307    -1.869808      22.18
 O       4.188078     0.985761    -0.432582     283.48
 H       5.167328     1.186286    -0.508522      22.29
 C       4.905001    -1.365449     0.134362      87.14
 H       4.871464    -1.124787     1.187147      24.41
 O       4.503796    -2.742520     0.142946     330.56
 H       4.534473    -3.065073    -0.763133      30.21
 C       6.444632    -1.270010    -0.325990      87.27
 O       6.979018     0.071117    -0.130380     308.77
 H       7.544218     0.092926     0.790714      23.74
 H       6.406638    -1.455754    -1.416732      30.43
 H       6.936223    -2.076310     0.222718      28.96
55
name= lig-ACN-Water-frame_36
 C      -3.944100    -0.337335    -3.062248      63.78
 H      -4.014135    -1.390599    -3.427302      24.67
 C      -3.661249     1.151638    -1.205143      54.14
 H      -3.544954     1.284104    -0.125709      20.47
 C      -3.686040     2.233609    -2.116395      26.04
 O      -3.529029     3.536342    -1.764020     235.16
 C      -3.936027     4.061794    -0.434872     104.02
 H      -3.603097     3.556453     0.466389      31.12
 H      -5.072044     4.076073    -0.317831      25.37
 H      -3.541486     5.011922    -0.450475      27.84
 C      -3.884575     2.061984    -3.499256       5.26
 O      -3.804474     3.098042    -4.452362      57.43
 H      -3.992768     3.975611    -3.915414      24.32
 C      -3.908435     0.712447    -4.007869      59.13
 H      -3.965269     0.507092    -5.151307      22.40
 C      -3.853189    -0.130501    -1.722188      36.39
 C      -3.989242    -1.413535    -0.787295      71.26
 H      -4.687686    -2.125056    -1.263604      24.50
 O      -4.689785    -1.120333     0.450056     162.82
 H      -4.059380    -0.622629     1.065711      23.19
 C      -2.570453    -2.085223    -0.631821      94.47
 H      -2.161532    -2.344311    -1.651798      25.04
 C      -2.723169    -3.446263     0.177311     109.21
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 O      -3.468171    -4.477222    -0.595856     198.09
 H      -3.060560    -4.527390    -1.453913      31.49
 H      -3.342087    -3.184231     1.068979      25.79
 H      -1.676649    -3.695082     0.482398      26.74
 C       1.742327    -1.503922    -1.421866      43.53
 H       2.231388    -1.944468    -2.265200      18.72
 C       1.855008    -0.253272     0.644813      42.23
 H       2.295839     0.522284     1.386917      23.88
 C       0.497875    -0.493617     0.964796      -7.44
 O      -0.234388    -0.008720     2.026620     174.71
 C       0.546339     0.839726     2.953508     105.97
 H      -0.159440     1.320831     3.663849      24.63
 H       1.320154     0.148581     3.466882      22.49
 H       0.973042     1.710752     2.406321      24.47
 C      -0.290208    -1.193803    -0.046310      -2.87
 O      -1.715669    -1.145458     0.111070     152.73
 C       0.323182    -1.687885    -1.210634      68.04
 H      -0.283125    -2.264691    -1.959329      22.06
 C       2.491771    -0.709516    -0.557550      42.86
 C       3.954864    -0.431887    -0.797506      97.20
 H       4.300362    -0.560704    -1.850212      22.16
 O       4.232434     0.949229    -0.410582     268.53
 H       5.252093     1.023572    -0.537632      19.01
 C       4.944538    -1.399980     0.120375      78.53
 H       4.781508    -1.013469     1.090535      26.38
 O       4.545332    -2.790115     0.084357     348.05
 H       4.638908    -3.087135    -0.882324      28.02
 C       6.407191    -1.288785    -0.291129     110.99
 O       7.021250     0.080150    -0.219145     286.74
 H       7.654903     0.084885     0.636432      24.04
 H       6.557953    -1.566390    -1.345963      30.48
 H       7.073315    -1.925351     0.247543      28.92
55
name= lig-ACN-Water-frame_37
 C      -3.954865    -0.342301    -3.143427      41.18
 H      -4.193410    -1.325814    -3.615520      20.64
 C      -3.695584     1.139214    -1.260681      46.06
 H      -3.653295     1.435375    -0.151707      19.51
 C      -3.722576     2.229596    -2.130992      25.65
 O      -3.507047     3.550945    -1.734790     218.96
 C      -3.874075     3.994881    -0.413491     101.96
 H      -3.442811     3.332659     0.239254      28.99
 H      -5.020029     3.967389    -0.299940      23.26
 H      -3.515645     4.989392    -0.289424      25.28
 C      -3.859341     2.034424    -3.590885      24.36
 O      -3.757505     3.102021    -4.514766     113.67
 H      -3.764586     3.973745    -4.083975      25.89
 C      -4.008400     0.742481    -4.001128      66.07
 H      -3.912890     0.541106    -5.128548      22.57
 C      -3.831942    -0.203340    -1.697326      24.49
 C      -3.928380    -1.376918    -0.834673      88.37
 H      -4.452203    -2.207294    -1.372315      26.27
 O      -4.700515    -1.050290     0.449953     146.11
 H      -4.077981    -0.657436     1.058567      25.28
 C      -2.615756    -2.081339    -0.596283      91.71
 H      -2.235204    -2.215284    -1.620528      27.86
 C      -2.750398    -3.442309     0.150523     116.67
 O      -3.481442    -4.479899    -0.550698     197.03
 H      -2.957096    -4.678263    -1.389887      29.22
 H      -3.220693    -3.386967     1.145762      26.71
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 H      -1.731382    -3.914909     0.326482      26.25
 C       1.709210    -1.496738    -1.394683      54.61
 H       2.212665    -1.999048    -2.209498      25.26
 C       1.867583    -0.177324     0.636901      -5.48
 H       2.630946     0.352355     1.306730      22.12
 C       0.503332    -0.467066     0.861067      -0.50
 O      -0.178068    -0.076440     2.054487     180.21
 C       0.531799     0.866086     2.968735     110.22
 H      -0.207709     1.271355     3.720811      26.15
 H       1.308886     0.249817     3.587071      26.05
 H       1.116356     1.580520     2.408467      28.67
 C      -0.297770    -1.175838    -0.080130      22.00
 O      -1.624815    -1.213332     0.142093     148.05
 C       0.322685    -1.667489    -1.218074      80.38
 H      -0.308239    -2.223697    -2.003386      25.41
 C       2.495513    -0.718714    -0.495594     -29.10
 C       4.004702    -0.527540    -0.764756     115.10
 H       4.101902    -0.685270    -1.835640      21.86
 O       4.304372     0.930244    -0.399698     244.98
 H       5.264760     1.039120    -0.346157      20.68
 C       4.904154    -1.374559     0.081044      87.79
 H       4.785029    -1.155951     1.098350      25.71
 O       4.585942    -2.828696     0.009173     296.00
 H       4.807065    -3.153666    -0.964219      26.66
 C       6.468146    -1.291316    -0.297830     100.04
 O       7.001510     0.062716    -0.333249     268.91
 H       7.699138     0.190691     0.398432      23.73
 H       6.550570    -1.768835    -1.281610      29.89
 H       6.887349    -1.905632     0.448151      29.57
55
name= lig-ACN-Water-frame_38
 C      -4.020743    -0.404104    -3.178616      54.42
 H      -4.059388    -1.455219    -3.504963      28.34
 C      -3.756426     1.148689    -1.301633      48.98
 H      -3.701940     1.254923    -0.146937      22.32
 C      -3.745031     2.285273    -2.202809      24.68
 O      -3.481018     3.592111    -1.762538     243.51
 C      -3.802884     3.869233    -0.364572     105.86
 H      -3.295638     3.358097     0.340093      30.48
 H      -4.915615     3.796471    -0.153556      24.55
 H      -3.480776     4.940323    -0.255890      25.10
 C      -3.789515     2.107198    -3.571739      23.63
 O      -3.724815     3.089164    -4.536353     119.86
 H      -3.707091     3.941842    -4.101732      29.65
 C      -4.026400     0.739688    -4.093900      46.18
 H      -4.385520     0.598501    -5.143167      24.35
 C      -3.846778    -0.156025    -1.824982      29.50
 C      -3.941947    -1.350167    -0.761020      73.28
 H      -4.643848    -2.068906    -1.251161      24.00
 O      -4.678589    -1.037362     0.369432     170.95
 H      -4.156882    -0.484240     0.879579      29.88
 C      -2.555939    -2.124335    -0.554235      97.46
 H      -2.165319    -2.357645    -1.519485      28.36
 C      -2.700283    -3.483575     0.171269     114.30
 O      -3.511290    -4.461188    -0.546580     200.65
 H      -2.857057    -4.963110    -1.131251      27.98
 H      -3.184465    -3.254908     1.119890      26.95
 H      -1.604319    -3.790794     0.317465      26.40
 C       1.745613    -1.493401    -1.410896      69.57
 H       2.134562    -1.878878    -2.366640      26.63
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 C       1.872936    -0.152321     0.638206      29.69
 H       2.352120     0.341675     1.490132      29.72
 C       0.503702    -0.383823     0.886708     -20.41
 O      -0.097487    -0.102760     2.059919     169.21
 C       0.530960     0.802716     2.964436     118.43
 H      -0.394999     1.228618     3.456644      26.48
 H       1.254487     0.340513     3.726040      25.34
 H       0.940059     1.652456     2.456573      29.08
 C      -0.269934    -1.126156    -0.122421     -20.30
 O      -1.651209    -1.300856     0.207694     147.15
 C       0.360308    -1.682256    -1.259580      78.89
 H      -0.162452    -2.267116    -2.082768      27.44
 C       2.508187    -0.762794    -0.490690       6.61
 C       3.981921    -0.493563    -0.732849     145.20
 H       4.279790    -0.681566    -1.745176      26.41
 O       4.355333     0.866415    -0.409122     275.57
 H       5.317471     0.810611    -0.452082      20.82
 C       4.963999    -1.482149     0.076112      95.53
 H       4.817436    -1.210054     1.086170      28.12
 O       4.635622    -2.825639    -0.055026     312.77
 H       4.633807    -3.062322    -1.093600      25.29
 C       6.452644    -1.337401    -0.275943     112.02
 O       6.991247     0.063875    -0.433042     261.34
 H       7.530594     0.122035     0.374290      24.88
 H       6.723378    -1.813633    -1.212976      29.71
 H       7.079910    -1.745299     0.480314      29.68
55
name= lig-ACN-Water-frame_39
 C      -4.053221    -0.349214    -3.259112      51.53
 H      -4.173842    -1.321225    -3.689679      26.57
 C      -3.814818     1.202915    -1.394942      60.01
 H      -3.773422     1.413686    -0.291818      24.70
 C      -3.682036     2.311102    -2.184824      21.62
 O      -3.477317     3.602506    -1.773757     162.61
 C      -3.725267     3.807712    -0.314859     105.43
 H      -3.107408     3.215086     0.195639      33.84
 H      -4.772225     3.475518    -0.106497      28.52
 H      -3.619253     4.946271    -0.139489      25.96
 C      -3.786464     2.007084    -3.638082      11.43
 O      -3.691711     3.121266    -4.540683      24.10
 H      -3.846478     4.003051    -4.060231      25.32
 C      -4.032938     0.736240    -4.103143      76.66
 H      -4.229594     0.703150    -5.147397      24.13
 C      -3.884348    -0.150536    -1.846656      -5.26
 C      -3.924772    -1.376055    -0.887916      46.37
 H      -4.485213    -2.217584    -1.363607      23.11
 O      -4.677686    -1.000998     0.374619     147.51
 H      -4.172658    -0.362319     0.952342      25.72
 C      -2.544362    -2.157849    -0.595496      85.20
 H      -2.139026    -2.293473    -1.554189      27.24
 C      -2.666302    -3.492844     0.228581     107.33
 O      -3.505323    -4.438687    -0.534473     221.23
 H      -2.952227    -4.971383    -1.092334      28.98
 H      -3.167210    -3.380128     1.184460      25.99
 H      -1.661650    -3.987003     0.487868      25.57
 C       1.815459    -1.472432    -1.469671      51.71
 H       2.426423    -1.773985    -2.355853      20.48
 C       1.882221    -0.205458     0.634624      98.12
 H       2.501430     0.364724     1.245168      26.86
 C       0.507622    -0.409438     0.820710      -4.02
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 O      -0.085997    -0.141337     2.051125     181.92
 C       0.458577     0.819610     3.003611     113.50
 H      -0.308070     1.205944     3.726323      26.37
 H       1.220270     0.232926     3.608314      26.54
 H       1.043356     1.575715     2.492250      27.89
 C      -0.303704    -1.108984    -0.121868      -1.48
 O      -1.618169    -1.342043     0.285606     138.45
 C       0.369121    -1.657008    -1.251729      65.78
 H      -0.260103    -2.246407    -1.922237      26.34
 C       2.541794    -0.725497    -0.490857     -10.34
 C       4.039369    -0.528482    -0.742762     109.01
 H       4.103654    -0.666746    -1.789947      23.32
 O       4.402504     0.839725    -0.398767     286.00
 H       5.393446     0.895198    -0.570164      19.90
 C       5.001300    -1.496611     0.119974      93.11
 H       4.882830    -1.316378     1.173543      26.95
 O       4.639997    -2.895202    -0.092386     294.79
 H       4.760410    -3.135180    -1.124817      27.07
 C       6.526992    -1.371566    -0.285577      96.29
 O       6.965574     0.069971    -0.469175     243.05
 H       7.581734     0.368436     0.259500      24.98
 H       6.638749    -1.909651    -1.220491      31.93
 H       7.087899    -1.893085     0.491158      29.98
55
name= lig-ACN-Water-frame_40
 C      -4.062196    -0.330610    -3.265698      39.07
 H      -4.302090    -1.307781    -3.640994      24.97
 C      -3.817418     1.157950    -1.368728      52.61
 H      -3.889401     1.302671    -0.314188      21.73
 C      -3.628785     2.263649    -2.294182      16.63
 O      -3.493150     3.609993    -1.757271     223.82
 C      -3.666079     3.725380    -0.331438     112.64
 H      -2.840009     3.403926     0.185132      33.10
 H      -4.596910     3.325774     0.052394      29.15
 H      -3.638392     4.875936    -0.101458      26.06
 C      -3.778275     2.133750    -3.661745      29.50
 O      -3.679152     3.118921    -4.525729     116.06
 H      -3.800664     4.070625    -4.045781      18.86
 C      -4.011364     0.802796    -4.184569      60.49
 H      -3.932650     0.531330    -5.185186      24.24
 C      -3.935208    -0.171842    -1.871497      22.63
 C      -3.895756    -1.379046    -0.922708      66.36
 H      -4.547382    -2.138306    -1.401585      25.32
 O      -4.675213    -1.015331     0.320028     145.12
 H      -3.923944    -0.575399     0.973273      20.84
 C      -2.523939    -2.128151    -0.573682      87.87
 H      -2.030153    -2.382655    -1.471471      26.42
 C      -2.725494    -3.492062     0.213599     107.90
 O      -3.497813    -4.433918    -0.504654     228.54
 H      -2.894380    -4.620768    -1.281613      28.39
 H      -3.234602    -3.233758     1.134560      25.60
 H      -1.659314    -3.865840     0.347397      25.04
 C       1.771521    -1.416216    -1.455654      62.57
 H       2.099009    -1.990848    -2.349947      23.93
 C       1.934902    -0.235800     0.616861      45.71
 H       2.425886     0.271133     1.361949      27.00
 C       0.532416    -0.441250     0.869777     -23.86
 O      -0.177678    -0.139004     2.034160     171.22
 C       0.478806     0.771796     3.037541     108.92
 H      -0.431666     1.079606     3.591135      25.09
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 H       1.201687     0.261476     3.688129      24.53
 H       0.882510     1.690565     2.555971      26.02
 C      -0.257668    -1.149260    -0.115717     -12.97
 O      -1.593813    -1.359721     0.286622     149.44
 C       0.426958    -1.621666    -1.266049      87.26
 H      -0.016876    -2.209447    -2.011096      26.68
 C       2.589833    -0.725421    -0.565647      40.17
 C       4.114787    -0.571371    -0.722924     107.92
 H       4.445318    -0.778907    -1.702708      24.44
 O       4.432306     0.869679    -0.389851     265.03
 H       5.453858     0.898556    -0.496050      19.14
 C       5.013406    -1.532428     0.081896      85.56
 H       4.840706    -1.302243     1.154594      25.84
 O       4.645902    -2.954726    -0.067430     315.90
 H       4.731214    -3.161003    -1.075817      26.26
 C       6.560449    -1.356993    -0.297711     101.51
 O       6.969011     0.044320    -0.476738     253.01
 H       7.568618     0.155390     0.366977      23.86
 H       6.732863    -1.769327    -1.291957      30.46
 H       7.273404    -1.824764     0.430842      29.01
55
name= lig-ACN-Water-frame_41
55
name= lig-ACN-Water-frame_42
 C      -4.024985    -0.321735    -3.352804      30.84
 H      -4.300967    -1.331043    -3.792939      27.18
 C      -3.686837     1.106858    -1.359368      49.21
 H      -3.461626     1.204860    -0.328228      26.34
 C      -3.711348     2.215055    -2.266254      27.96
 O      -3.542502     3.505924    -1.745094     258.57
 C      -3.551233     3.712879    -0.340584     114.66
 H      -2.527720     3.505773     0.052712      27.05
 H      -4.362074     3.210532     0.156493      25.82
 H      -3.661450     4.775759    -0.094061      25.53
 C      -3.709962     2.151354    -3.663949      37.75
 O      -3.657094     3.140450    -4.574937       8.12
 H      -3.802024     4.173536    -4.192669      21.89
 C      -3.899110     0.865371    -4.183079      41.62
 H      -4.157177     0.654190    -5.237451      26.62
 C      -3.864978    -0.196821    -1.908981      -5.78
 C      -3.853700    -1.379999    -0.982678      63.04
 H      -4.441180    -2.174405    -1.478801      26.11
 O      -4.655884    -1.125408     0.320188      84.84
 H      -4.038771    -0.551015     0.811069      31.57
 C      -2.536175    -2.058187    -0.655934      88.88
 H      -2.072399    -2.348679    -1.635761      28.26
 C      -2.800701    -3.401890     0.193498     106.67
 O      -3.507929    -4.437174    -0.554823     185.80
 H      -2.808963    -4.728667    -1.200910      28.44
 H      -3.515612    -3.032594     0.954713      27.33
 H      -1.836203    -3.754236     0.562824      27.75
 C       1.817723    -1.418725    -1.504746      57.96
 H       2.231264    -1.651818    -2.483238      19.70
 C       1.980677    -0.310493     0.698515      74.06
 H       2.573117     0.333074     1.399580      26.06
 C       0.579949    -0.546674     0.934634     -17.52
 O      -0.213712    -0.052214     1.953273     188.12
 C       0.427492     0.658249     3.061949     115.57
 H      -0.368737     0.813539     3.785684      26.03
 H       1.172258     0.025179     3.472214      26.04
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 H       0.892785     1.651306     2.735326      25.95
 C      -0.199286    -1.248229    -0.077191      -9.71
 O      -1.570823    -1.277306     0.190675     137.63
 C       0.439824    -1.635152    -1.292092      82.11
 H      -0.196488    -2.040014    -2.064276      29.93
 C       2.567153    -0.755530    -0.491277      34.26
 C       4.096269    -0.529018    -0.751911     109.88
 H       4.338006    -0.740994    -1.771059      26.04
 O       4.467587     0.841171    -0.366072     284.26
 H       5.427197     0.841821    -0.311491      21.62
 C       5.071924    -1.511446     0.061735      79.15
 H       4.965946    -1.274721     1.193375      25.35
 O       4.684447    -2.957037    -0.035972     295.85
 H       4.764223    -3.134819    -0.978743      31.02
 C       6.579558    -1.456332    -0.359297      94.94
 O       7.035678     0.004513    -0.423083     281.83
 H       7.697955     0.011677     0.392221      24.88
 H       6.660482    -1.757594    -1.430446      29.18
 H       7.292109    -2.049649     0.317722      28.52
55
name= lig-ACN-Water-frame_43
 C      -3.964121    -0.298087    -3.317198      59.16
 H      -4.339057    -1.253375    -3.790755      17.98
 C      -3.599404     1.084458    -1.445215      67.03
 H      -3.414313     1.271328    -0.365599      25.03
 C      -3.670006     2.254284    -2.213683      18.24
 O      -3.583629     3.543254    -1.744707     217.21
 C      -3.501275     3.747532    -0.290517     118.17
 H      -2.530858     3.339962     0.212562      27.26
 H      -4.264179     3.208134     0.263743      26.65
 H      -3.614578     4.785542    -0.293862      27.28
 C      -3.716967     2.065781    -3.654299      15.48
 O      -3.644147     3.097463    -4.589892     108.21
 H      -3.577938     4.027400    -4.043102      19.88
 C      -3.935343     0.769472    -4.176399      53.60
 H      -3.877254     0.774297    -5.315704      24.82
 C      -3.784364    -0.194089    -1.962077      53.20
 C      -3.880832    -1.412692    -1.019040      74.00
 H      -4.500868    -2.193953    -1.477811      26.76
 O      -4.620346    -1.164039     0.313798      51.33
 H      -4.336032    -0.436862     0.796846      31.32
 C      -2.469806    -2.129990    -0.692476      86.00
 H      -1.931091    -2.387839    -1.677975      27.62
 C      -2.841733    -3.351410     0.156533     122.20
 O      -3.468227    -4.408354    -0.570948     186.10
 H      -2.871014    -4.900736    -1.139370      27.93
 H      -3.487173    -3.127939     1.038761      27.47
 H      -1.943536    -3.704094     0.640770      28.77
 C       1.831192    -1.378962    -1.466893      55.93
 H       2.298774    -1.700200    -2.382434      27.21
 C       1.932492    -0.381949     0.761817       6.82
 H       2.474133     0.305679     1.531386      23.61
 C       0.561448    -0.570461     0.902226      10.60
 O      -0.211503    -0.009578     1.902829     184.97
 C       0.463653     0.585794     3.097852     113.43
 H      -0.370434     0.732028     3.777365      26.95
 H       1.237653     0.018217     3.551019      27.89
 H       0.811948     1.627306     2.828903      27.45
 C      -0.176016    -1.251828    -0.113635     -14.68
 O      -1.622031    -1.209148     0.110154     119.18
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 C       0.447651    -1.654943    -1.292170      70.00
 H       0.007095    -2.114996    -2.213895      26.51
 C       2.605757    -0.802972    -0.467757      14.04
 C       4.061580    -0.572815    -0.707428     115.80
 H       4.167838    -0.613289    -1.792475      20.96
 O       4.465378     0.835210    -0.347418     256.73
 H       5.452432     0.719924    -0.488780      21.08
 C       5.052801    -1.511148     0.040535      81.40
 H       4.976012    -1.169868     1.159081      24.54
 O       4.707108    -2.897084    -0.060169     302.26
 H       4.775318    -3.140778    -1.048521      28.62
 C       6.568709    -1.418974    -0.434101      99.28
 O       7.052507    -0.087557    -0.428724     292.08
 H       7.556386     0.207240     0.425618      22.67
 H       6.668977    -1.882838    -1.471820      29.68
 H       7.174666    -2.106149     0.250080      29.03
55
name= lig-ACN-Water-frame_44
 C      -3.991184    -0.404641    -3.349035      44.48
 H      -4.032019    -1.454344    -3.690752      29.04
 C      -3.499117     1.126003    -1.425245      55.77
 H      -3.469965     1.185555    -0.279510      23.47
 C      -3.579903     2.256901    -2.238281      10.83
 O      -3.618264     3.577881    -1.734472     209.60
 C      -3.481152     3.794662    -0.260145     110.65
 H      -2.431867     3.332322     0.055056      27.53
 H      -4.383687     3.373850     0.211728      27.43
 H      -3.441165     4.784358    -0.004140      29.00
 C      -3.755572     2.037832    -3.644593      26.51
 O      -3.612981     3.064069    -4.575040      85.33
 H      -3.760021     4.057981    -4.225897      21.03
 C      -3.900309     0.752020    -4.193299      54.67
 H      -4.089442     0.545039    -5.308950      24.07
 C      -3.732840    -0.207204    -1.913677      -7.57
 C      -3.855064    -1.426590    -0.977876      93.54
 H      -4.423045    -2.192875    -1.506515      25.75
 O      -4.573284    -1.195347     0.212130     139.07
 H      -4.143458    -0.309106     0.615805      25.93
 C      -2.502078    -2.121291    -0.695411      90.10
 H      -2.066179    -2.506034    -1.708733      23.70
 C      -2.757435    -3.362564     0.199633     109.61
 O      -3.481496    -4.404243    -0.575463     226.83
 H      -2.840334    -4.546341    -1.350224      27.79
 H      -3.514429    -2.994017     0.912772      25.02
 H      -1.851365    -3.729937     0.624277      27.20
 C       1.866435    -1.404559    -1.437657      55.10
 H       2.428381    -1.718050    -2.301765      25.59
 C       1.924014    -0.439223     0.767218      62.00
 H       2.553169    -0.019227     1.658609      21.84
 C       0.510084    -0.567157     0.867075      -1.89
 O      -0.191578     0.026881     1.913105     206.43
 C       0.436016     0.534372     3.097479     121.21
 H      -0.284754     0.597242     3.916668      26.72
 H       1.201992    -0.174300     3.376811      26.60
 H       0.953355     1.490956     2.876429      27.46
 C      -0.301051    -1.212744    -0.155921      -2.96
 O      -1.627616    -1.182383    -0.016510     160.61
 C       0.452948    -1.670896    -1.310843      79.59
 H      -0.256547    -2.219354    -2.022928      25.27
 C       2.612068    -0.806838    -0.363038      14.56
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 C       4.095488    -0.543117    -0.699965     115.88
 H       4.253239    -0.741493    -1.796570      22.15
 O       4.454230     0.817573    -0.340575     269.36
 H       5.436692     0.949734    -0.563544      21.66
 C       5.077819    -1.527183     0.021404      92.40
 H       5.077517    -1.358902     1.172105      25.57
 O       4.696745    -2.886215    -0.102297     284.32
 H       4.653594    -3.082625    -1.136175      27.22
 C       6.481694    -1.437360    -0.475355     102.34
 O       7.093519    -0.093425    -0.477804     266.96
 H       7.607490     0.027516     0.337617      24.96
 H       6.560218    -1.797005    -1.563045      29.30
 H       7.084622    -2.080863     0.222210      28.57
55
name= lig-ACN-Water-frame_45
 C      -3.941776    -0.412466    -3.267948      65.73
 H      -4.222175    -1.355497    -3.672269      23.64
 C      -3.469815     1.079264    -1.369680      51.50
 H      -3.297862     1.330646    -0.268252      23.60
 C      -3.537206     2.244077    -2.232643       2.65
 O      -3.622901     3.613394    -1.729938     173.04
 C      -3.481831     3.791784    -0.303443     117.17
 H      -2.559848     3.180125     0.194861      28.23
 H      -4.316920     3.406215     0.338187      27.73
 H      -3.340698     4.820948    -0.293425      29.49
 C      -3.729855     2.052317    -3.664617       2.75
 O      -3.613168     3.075228    -4.580965      28.07
 H      -3.732094     3.964317    -4.134420      24.61
 C      -3.903813     0.686682    -4.149908      35.45
 H      -4.196322     0.675579    -5.233709      23.44
 C      -3.716261    -0.207994    -1.927545      38.80
 C      -3.805423    -1.434102    -1.049189      83.62
 H      -4.422114    -2.157400    -1.582511      27.05
 O      -4.560881    -1.146750     0.163018     108.86
 H      -4.041386    -0.607825     0.914755      24.38
 C      -2.519074    -2.150641    -0.713633      89.63
 H      -2.077193    -2.428920    -1.755743      28.14
 C      -2.723789    -3.398059     0.222226     118.34
 O      -3.462077    -4.346880    -0.552792     190.51
 H      -2.948400    -4.680006    -1.382804      25.46
 H      -3.253858    -3.206951     1.160690      27.89
 H      -1.754619    -3.752524     0.530829      28.89
 C       1.835210    -1.484550    -1.387158      54.72
 H       2.224881    -1.777604    -2.360849      21.95
 C       1.894145    -0.479920     0.824099      13.38
 H       2.406529    -0.074026     1.750142      29.06
 C       0.480446    -0.512303     0.877253     -11.76
 O      -0.273167     0.036891     1.904443     189.52
 C       0.500598     0.451918     3.100992     115.06
 H      -0.340902     0.603440     3.814580      26.85
 H       1.178946    -0.318239     3.491593      28.53
 H       0.948661     1.423680     3.003719      28.01
 C      -0.228294    -1.136388    -0.219026      -3.79
 O      -1.671817    -1.143466    -0.105371     136.76
 C       0.456755    -1.664368    -1.276483      86.63
 H       0.123676    -2.183843    -2.223741      26.52
 C       2.605344    -0.841044    -0.429261       4.48
 C       4.107686    -0.555398    -0.646583     107.03
 H       4.271560    -0.645359    -1.779531      25.70
 O       4.438029     0.856895    -0.345404     266.00
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 H       5.412043     0.806785    -0.501873      23.32
 C       5.054365    -1.520445     0.056747      86.64
 H       4.995506    -1.271237     1.178089      26.90
 O       4.641845    -2.950256    -0.173913     280.31
 H       4.640118    -3.128796    -1.189452      27.88
 C       6.537257    -1.459410    -0.512390     100.15
 O       7.108615    -0.088018    -0.541790     231.44
 H       7.600954     0.138028     0.216217      25.54
 H       6.423733    -1.754590    -1.616946      30.30
 H       7.206952    -2.215065    -0.077166      31.19
55
name= lig-ACN-Water-frame_46
 C      -3.919959    -0.330227    -3.270700      49.31
 H      -4.251277    -1.284183    -3.575052      23.43
 C      -3.473103     1.113996    -1.397567      67.63
 H      -3.296419     1.108351    -0.315821      24.68
 C      -3.569490     2.229824    -2.192154      27.47
 O      -3.590729     3.513596    -1.781039     207.49
 C      -3.477762     3.796546    -0.338799     112.20
 H      -2.508943     3.253328     0.102990      25.36
 H      -4.477158     3.551001     0.106609      25.48
 H      -3.352085     4.865434    -0.143019      26.40
 C      -3.638912     2.015700    -3.609116      27.28
 O      -3.651728     3.106335    -4.578126     185.14
 H      -3.587002     3.975823    -4.203294      24.28
 C      -3.930152     0.766456    -4.118211      66.11
 H      -4.074967     0.539054    -5.152520      24.86
 C      -3.651084    -0.189226    -1.872278      22.88
 C      -3.849780    -1.445946    -1.054229      83.68
 H      -4.483004    -2.166613    -1.578996      27.43
 O      -4.587910    -1.095032     0.187615     149.24
 H      -3.922158    -0.896996     0.773049      31.18
 C      -2.446367    -2.166848    -0.735590      88.87
 H      -1.948209    -2.660197    -1.626004      25.49
 C      -2.643085    -3.392346     0.176163     110.65
 O      -3.483349    -4.338592    -0.525058     194.15
 H      -2.830853    -4.869907    -1.036180      28.53
 H      -3.175177    -3.160593     1.092248      27.82
 H      -1.690280    -3.852775     0.371590      27.15
 C       1.877423    -1.536583    -1.409592      59.54
 H       2.468900    -1.888409    -2.276396      20.61
 C       1.895764    -0.488331     0.784231      68.17
 H       2.502106     0.035731     1.497714      25.34
 C       0.461999    -0.477187     0.845290      -0.38
 O      -0.312865     0.021274     1.900865     195.40
 C       0.463201     0.396411     3.136249     105.57
 H      -0.241080     0.625245     3.973494      25.58
 H       1.123703    -0.475612     3.418893      26.62
 H       1.115244     1.175393     2.835680      26.10
 C      -0.282252    -1.081721    -0.208722       5.28
 O      -1.633919    -1.069290    -0.129525     175.74
 C       0.453016    -1.681974    -1.312986      63.17
 H      -0.262956    -2.080987    -2.042087      25.07
 C       2.574433    -0.849413    -0.355253      26.15
 C       4.047626    -0.558782    -0.651624      74.22
 H       4.190082    -0.745000    -1.799950      21.70
 O       4.420675     0.863016    -0.332871     264.60
 H       5.369106     0.949423    -0.374080      23.88
 C       5.071736    -1.643551     0.058493      84.54
 H       5.051813    -1.578989     1.172758      26.08
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 O       4.596986    -2.952343    -0.202019     331.92
 H       4.626228    -3.125604    -1.180569      29.34
 C       6.558703    -1.449270    -0.566357     102.06
 O       7.088006    -0.120419    -0.548100     274.29
 H       7.528149     0.105982     0.284802      27.75
 H       6.478867    -1.709997    -1.663413      30.71
 H       7.234396    -2.121650    -0.053271      30.06
55
name= lig-ACN-Water-frame_47
 C      -3.942394    -0.316391    -3.262274      70.57
 H      -4.004453    -1.270767    -3.747077      24.88
 C      -3.467329     1.090513    -1.304560      53.91
 H      -3.483836     1.357236    -0.295273      21.45
 C      -3.573739     2.187409    -2.232870      16.64
 O      -3.518763     3.523387    -1.791958     233.53
 C      -3.512135     3.791770    -0.397327     111.73
 H      -2.666673     3.218137     0.191579      24.00
 H      -4.421573     3.410701     0.160130      24.66
 H      -3.356071     4.934964    -0.420277      24.09
 C      -3.619789     2.123721    -3.646030      20.89
 O      -3.682377     3.102688    -4.515410     157.70
 H      -3.850742     3.984483    -4.154763      25.70
 C      -3.897053     0.821747    -4.142833      32.85
 H      -4.105865     0.808405    -5.165224      24.96
 C      -3.652499    -0.212140    -1.914606      16.88
 C      -3.823960    -1.451406    -0.992200      84.65
 H      -4.460118    -2.166629    -1.540735      25.48
 O      -4.578140    -1.104830     0.206701     147.76
 H      -4.062041    -0.570298     0.865235      25.02
 C      -2.443975    -2.106551    -0.755815      96.81
 H      -2.108939    -2.224780    -1.801729      26.94
 C      -2.580957    -3.368384     0.166729     109.55
 O      -3.484577    -4.378213    -0.489627     216.42
 H      -2.992009    -4.876218    -1.149934      29.15
 H      -3.082839    -2.977733     1.050000      27.19
 H      -1.651193    -3.810677     0.566756      26.86
 C       1.842868    -1.554247    -1.399244      53.56
 H       2.353915    -2.037675    -2.261767      21.02
 C       1.860921    -0.368448     0.773324      44.92
 H       2.351542     0.107971     1.538231      23.89
 C       0.460514    -0.471336     0.857929       9.01
 O      -0.308851     0.006350     1.931688     214.34
 C       0.440975     0.323919     3.096587     119.65
 H      -0.312897     0.731679     3.832999      25.08
 H       0.891580    -0.640773     3.507056      25.16
 H       1.139297     1.126598     3.030093      26.06
 C      -0.229636    -1.102952    -0.241831       7.66
 O      -1.650980    -1.045727    -0.131910     168.64
 C       0.439762    -1.643641    -1.319590      71.66
 H       0.027042    -2.174674    -2.124559      24.03
 C       2.568434    -0.909501    -0.401496      29.47
 C       4.070852    -0.593625    -0.594714      95.06
 H       4.233467    -0.666326    -1.772265      19.04
 O       4.351757     0.808920    -0.303351     275.14
 H       5.340338     0.808393    -0.527460      20.71
 C       5.091314    -1.657367    -0.036630      98.09
 H       5.159255    -1.459257     1.030268      26.55
 O       4.565590    -2.997161    -0.215900     364.24
 H       4.522946    -3.170555    -1.174707      30.66
 C       6.506608    -1.514596    -0.578340     109.97
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 O       7.055167    -0.109148    -0.485677     269.00
 H       7.532441    -0.009650     0.462337      25.61
 H       6.586356    -1.798845    -1.634533      31.71
 H       7.165025    -2.183802    -0.055344      30.45
55
name= lig-ACN-Water-frame_48
 C      -3.894799    -0.296597    -3.325964      46.68
 H      -4.060301    -1.305702    -3.775917      26.53
 C      -3.537900     1.086797    -1.367629      60.24
 H      -3.459796     1.149790    -0.339590      25.00
 C      -3.491466     2.225454    -2.177963      15.15
 O      -3.443384     3.543846    -1.815801     224.44
 C      -3.542558     3.797517    -0.401301     108.20
 H      -2.624945     3.426990     0.153910      28.78
 H      -4.554635     3.499001     0.004983      27.64
 H      -3.561870     4.985959    -0.227858      25.99
 C      -3.708356     2.066817    -3.597769      15.63
 O      -3.712391     3.214947    -4.512575      44.93
 H      -3.780846     4.104634    -4.026184      19.65
 C      -3.847836     0.800814    -4.180846      70.85
 H      -4.117357     0.692703    -5.183887      29.54
 C      -3.740172    -0.196390    -1.888216      25.17
 C      -3.812184    -1.391107    -0.966999      83.46
 H      -4.381430    -2.237848    -1.402905      24.98
 O      -4.562790    -1.132247     0.248534      94.95
 H      -4.068178    -0.301476     0.746110      24.42
 C      -2.453617    -2.041175    -0.780973      97.35
 H      -2.051680    -2.377384    -1.721978      26.91
 C      -2.608937    -3.329142     0.126714     109.03
 O      -3.415000    -4.388178    -0.414607     217.75
 H      -2.961440    -4.648735    -1.278434      28.30
 H      -3.157905    -3.095875     1.051683      25.80
 H      -1.571840    -3.709609     0.348256      26.00
 C       1.840683    -1.566344    -1.370163      50.36
 H       2.327445    -1.981657    -2.276056      21.95
 C       1.870323    -0.281807     0.695129      57.20
 H       2.430876     0.159124     1.443038      23.66
 C       0.460036    -0.490765     0.823109      13.56
 O      -0.286812    -0.012783     1.887673     203.43
 C       0.402584     0.286277     3.163870     108.46
 H      -0.425336     0.688910     3.792376      25.17
 H       0.868001    -0.605150     3.710884      25.08
 H       1.211631     0.984679     2.945295      26.03
 C      -0.286977    -1.107130    -0.213954      14.18
 O      -1.629416    -1.064252    -0.107508     180.08
 C       0.429667    -1.650468    -1.353380      58.52
 H      -0.116286    -2.112149    -2.100902      23.51
 C       2.576771    -0.876014    -0.356910      19.62
 C       4.047142    -0.656031    -0.671421     101.19
 H       4.150389    -0.720255    -1.854155      21.93
 O       4.312423     0.739057    -0.247708     242.61
 H       5.278397     0.985823    -0.472010      18.70
 C       5.051785    -1.623787    -0.036251      96.60
 H       5.064103    -1.483728     1.016500      27.00
 O       4.558787    -3.039042    -0.214571     286.92
 H       4.529701    -3.203022    -1.181393      30.00
 C       6.536672    -1.549907    -0.597351      97.94
 O       6.995066    -0.142401    -0.420468     307.98
 H       7.393949     0.151823     0.571859      22.11
 H       6.570748    -1.720058    -1.648521      31.21
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 H       7.094787    -2.286762    -0.042262      29.88
55
name= lig-ACN-Water-frame_49
 C      -3.848079    -0.365769    -3.332521      57.52
 H      -4.092986    -1.403071    -3.703557      22.13
 C      -3.600377     1.131586    -1.391330      56.80
 H      -3.355313     1.219567    -0.347575      27.32
 C      -3.486447     2.257631    -2.242784      21.25
 O      -3.341729     3.592631    -1.789546     220.66
 C      -3.593349     3.859738    -0.366065      99.76
 H      -2.824906     3.415235     0.289582      30.48
 H      -4.518910     3.289802    -0.088953      28.03
 H      -3.646144     5.080826    -0.319849      25.75
 C      -3.752339     2.156700    -3.646287       1.81
 O      -3.727688     3.176300    -4.458213      -3.67
 H      -3.880762     4.135098    -4.089658      18.09
 C      -3.842372     0.787711    -4.191178      40.20
 H      -3.928772     0.640026    -5.265044      23.58
 C      -3.854684    -0.157456    -1.968511      47.45
 C      -3.885844    -1.372744    -1.026949      81.13
 H      -4.557264    -2.097191    -1.552103      27.05
 O      -4.522653    -1.119387     0.292076     106.34
 H      -3.969968    -0.510379     0.916433      25.44
 C      -2.488878    -2.061928    -0.745289     100.07
 H      -2.074620    -2.302300    -1.682467      29.52
 C      -2.605618    -3.268584     0.145864     118.99
 O      -3.347678    -4.391572    -0.404029     231.06
 H      -2.817232    -4.836568    -1.156429      26.69
 H      -2.957024    -2.969789     1.171523      27.26
 H      -1.533195    -3.603263     0.297096      26.01
 C       1.822345    -1.569149    -1.371744      40.25
 H       2.428478    -1.925381    -2.206262      19.78
 C       1.880298    -0.268545     0.669214      58.38
 H       2.377213     0.412252     1.362752      24.41
 C       0.511774    -0.468982     0.800779       2.58
 O      -0.264524    -0.033989     1.878062     190.87
 C       0.354034     0.288930     3.201437     105.76
 H      -0.376604     0.782820     3.865877      25.50
 H       0.743120    -0.683026     3.572243      25.99
 H       1.176331     1.072410     3.131956      24.39
 C      -0.243843    -1.134172    -0.240428       3.07
 O      -1.644143    -1.090173    -0.055417     162.51
 C       0.397801    -1.662492    -1.316988      79.01
 H      -0.132223    -2.014036    -2.166403      25.91
 C       2.547909    -0.873711    -0.436201      28.49
 C       4.009087    -0.630845    -0.736611     106.07
 H       4.194961    -0.700684    -1.908921      20.69
 O       4.311214     0.705091    -0.209638     265.11
 H       5.251724     0.755216    -0.445564      21.73
 C       5.020336    -1.730109    -0.027736      87.63
 H       4.964051    -1.488304     0.997405      28.55
 O       4.579978    -3.031428    -0.195209     320.03
 H       4.602629    -3.186909    -1.197531      29.45
 C       6.493203    -1.499918    -0.539128     111.02
 O       6.944407    -0.175362    -0.396271     328.22
 H       7.541361    -0.071527     0.489282      25.52
 H       6.502742    -1.712054    -1.575862      32.66
 H       7.236759    -2.175682    -0.120177      29.64
55
name= lig-ACN-Water-frame_50
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 C      -3.889715    -0.321652    -3.362453      44.11
 H      -3.759997    -1.311608    -3.868131      22.99
 C      -3.632129     1.187814    -1.442345      43.09
 H      -3.574981     1.377227    -0.324065      20.06
 C      -3.574155     2.315070    -2.260604      16.18
 O      -3.222942     3.617413    -1.749184     212.08
 C      -3.649525     3.859034    -0.366777     104.70
 H      -2.864673     3.641810     0.325592      28.05
 H      -4.653614     3.488809    -0.032862      26.49
 H      -3.808029     5.076863    -0.322939      25.09
 C      -3.729271     2.062107    -3.642966      18.11
 O      -3.746295     3.187090    -4.522841     -43.49
 H      -3.964177     4.003568    -3.905000      24.02
 C      -3.831938     0.796631    -4.177982      58.26
 H      -3.894399     0.832850    -5.308147      25.00
 C      -3.870181    -0.126962    -1.931133       0.74
 C      -3.953710    -1.364022    -1.007207      85.92
 H      -4.605357    -2.190448    -1.398375      23.17
 O      -4.486508    -1.077813     0.305651     141.02
 H      -3.830614    -0.641524     0.780084      27.21
 C      -2.566005    -2.030562    -0.798442      89.57
 H      -2.139441    -2.275972    -1.724139      27.70
 C      -2.522063    -3.293273     0.188936      99.86
 O      -3.306164    -4.387858    -0.399942     217.71
 H      -2.657950    -4.954203    -0.833464      28.32
 H      -3.168762    -3.035032     1.085758      26.00
 H      -1.464573    -3.594324     0.501913      25.75
 C       1.789289    -1.599598    -1.468381      40.86
 H       2.138536    -2.063157    -2.379820      18.19
 C       1.907833    -0.271424     0.644924      54.38
 H       2.499175     0.420987     1.355155      21.25
 C       0.500213    -0.451743     0.839900      10.43
 O      -0.250846    -0.014602     1.897167     222.25
 C       0.330674     0.302390     3.167957     114.06
 H      -0.593574     0.581999     3.676713      24.16
 H       0.756379    -0.527668     3.741878      26.41
 H       1.145335     1.125714     3.096270      23.09
 C      -0.252958    -1.124662    -0.185364      -8.57
 O      -1.663226    -1.101956    -0.002126     129.11
 C       0.401280    -1.699479    -1.348049      63.91
 H      -0.109837    -2.219095    -2.198761      22.03
 C       2.542189    -0.832657    -0.508177      35.92
 C       4.035338    -0.633000    -0.689830     104.31
 H       4.245884    -0.589518    -1.842180      20.24
 O       4.357812     0.683544    -0.213798     293.29
 H       5.311912     0.832978    -0.227625      20.11
 C       4.971492    -1.666876    -0.003120      84.42
 H       4.913543    -1.543496     1.051020      26.71
 O       4.592826    -3.098891    -0.212237     314.63
 H       4.613255    -3.286251    -1.236951      27.66
 C       6.423529    -1.544088    -0.514062     101.65
 O       6.930885    -0.123691    -0.397414     332.35
 H       7.498312     0.084693     0.405949      29.28
 H       6.448031    -1.750173    -1.551361      32.48
 H       7.006155    -2.276216     0.065920      29.54
55
name= lig-ACN-Water-frame_51
 C      -3.903721    -0.282900    -3.331252      55.68
 H      -3.930068    -1.317423    -3.676332      29.54
 C      -3.718817     1.180863    -1.416908      41.44
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 H      -3.761411     1.256000    -0.252580      19.21
 C      -3.605977     2.346896    -2.215624      27.86
 O      -3.180163     3.558963    -1.737597     238.08
 C      -3.685735     3.934968    -0.372624      94.45
 H      -3.007369     3.586365     0.373156      27.24
 H      -4.611248     3.316815    -0.298049      25.56
 H      -3.825473     5.115883    -0.378935      23.12
 C      -3.705159     2.195216    -3.657038      33.94
 O      -3.764975     3.170952    -4.571789      35.90
 H      -3.753274     4.182524    -4.252271      23.30
 C      -3.827706     0.837471    -4.213722      31.05
 H      -4.007898     0.591373    -5.329246      27.36
 C      -3.851287    -0.125127    -1.937611      25.53
 C      -3.920240    -1.357594    -0.928754      76.21
 H      -4.618140    -2.081378    -1.428364      24.60
 O      -4.490135    -1.000282     0.329558     198.32
 H      -3.913258    -0.523304     0.898392      24.12
 C      -2.495694    -2.054323    -0.760034      91.11
 H      -2.140813    -2.281765    -1.744757      26.88
 C      -2.583664    -3.291514     0.160124     109.17
 O      -3.245082    -4.424157    -0.387204     267.43
 H      -2.659667    -4.991653    -0.940222      28.37
 H      -3.054026    -2.948697     1.140899      24.43
 H      -1.495286    -3.538200     0.407966      24.44
 C       1.787496    -1.564402    -1.524746      27.74
 H       2.411671    -1.962515    -2.306548      17.84
 C       1.876908    -0.306991     0.575847      59.77
 H       2.592574     0.120371     1.405999      21.72
 C       0.512830    -0.488137     0.802298      13.21
 O      -0.255457    -0.004616     1.883177     210.95
 C       0.297291     0.355873     3.193097     110.98
 H      -0.454099     0.719270     3.888182      24.13
 H       0.877018    -0.477166     3.539777      24.51
 H       0.946656     1.311767     3.031513      23.81
 C      -0.305259    -1.140871    -0.203318      15.48
 O      -1.670068    -1.101131    -0.009768     170.36
 C       0.343199    -1.707790    -1.295315      71.55
 H      -0.377165    -2.339809    -1.935929      20.78
 C       2.523987    -0.832192    -0.572610      29.73
 C       4.044731    -0.630080    -0.700422      85.23
 H       4.321752    -0.827788    -1.804719      18.69
 O       4.397761     0.721458    -0.191466     258.45
 H       5.416930     0.660913    -0.298892      14.95
 C       4.914821    -1.682509     0.025494      94.63
 H       4.839236    -1.529452     1.099019      24.29
 O       4.595752    -3.117479    -0.242778     330.46
 H       4.681804    -3.200520    -1.277038      25.66
 C       6.390788    -1.522158    -0.453777     105.93
 O       6.929875    -0.104609    -0.435892     357.07
 H       7.320650     0.033735     0.395913      32.96
 H       6.514581    -1.846249    -1.481938      31.02
 H       7.065139    -2.161297     0.165389      28.84
55
name= lig-ACN-Water-frame_52
 C      -3.888830    -0.258932    -3.307689      64.42
 H      -4.210314    -1.133348    -3.811719      23.74
 C      -3.812761     1.179402    -1.361171      46.19
 H      -3.678458     1.384613    -0.231545      22.14
 C      -3.578152     2.278904    -2.236951      14.82
 O      -3.181825     3.555682    -1.702247     257.17
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 C      -3.721166     3.937895    -0.441368     108.96
 H      -3.078126     3.664015     0.385834      30.49
 H      -4.760166     3.635591    -0.168534      29.24
 H      -3.795655     5.092402    -0.475579      25.69
 C      -3.735771     2.183675    -3.661382      10.63
 O      -3.750045     3.250550    -4.650282      71.48
 H      -3.861947     4.092258    -4.080409      23.09
 C      -3.859920     0.899164    -4.125044      53.23
 H      -4.107068     0.923320    -5.244696      25.61
 C      -3.836828    -0.122666    -1.888993      26.88
 C      -3.826954    -1.293941    -0.935290      75.94
 H      -4.483185    -2.123616    -1.290626      25.64
 O      -4.540492    -0.924858     0.362019     107.84
 H      -3.891823    -0.550251     0.972405      24.73
 C      -2.517943    -2.038802    -0.715793      97.39
 H      -2.074282    -2.297423    -1.699464      26.31
 C      -2.571195    -3.305084     0.157961     107.36
 O      -3.239500    -4.499480    -0.396150     235.05
 H      -2.581419    -4.793091    -1.129016      27.23
 H      -3.152346    -3.111655     1.099671      25.41
 H      -1.512445    -3.607110     0.426798      24.52
 C       1.703920    -1.511591    -1.523192      54.97
 H       1.998226    -1.994601    -2.445027      21.64
 C       1.853026    -0.374532     0.576280      50.13
 H       2.410221     0.146421     1.449263      22.60
 C       0.455435    -0.484205     0.789615      17.76
 O      -0.293471     0.004492     1.862707     213.21
 C       0.350030     0.436565     3.155472     105.53
 H      -0.542901     0.438999     3.765437      24.25
 H       0.986056    -0.322390     3.576792      26.10
 H       0.934802     1.392675     3.076694      25.07
 C      -0.281321    -1.132496    -0.213959      22.03
 O      -1.659466    -1.108728    -0.057965     177.61
 C       0.375943    -1.749676    -1.296251      78.68
 H      -0.065724    -2.330969    -2.202308      21.60
 C       2.517912    -0.820851    -0.598548      49.86
 C       3.993675    -0.632311    -0.739366      93.24
 H       4.262392    -0.507565    -1.814464      19.94
 O       4.417844     0.699761    -0.211950     265.88
 H       5.406717     0.809473    -0.429829      19.08
 C       4.919204    -1.751440     0.046667      77.51
 H       4.713199    -1.663887     1.143834      24.89
 O       4.585838    -3.063060    -0.282358     334.26
 H       4.752236    -3.228594    -1.249870      26.64
 C       6.437873    -1.466472    -0.360171      96.97
 O       6.911788    -0.127395    -0.477604     348.58
 H       7.479415     0.120518     0.214803      31.13
 H       6.461543    -1.903862    -1.387563      29.81
 H       7.124515    -2.061126     0.301728      27.20
55
name= lig-ACN-Water-frame_53
 C      -3.929946    -0.229331    -3.288918      58.67
 H      -3.957097    -1.211127    -3.700305      27.77
 C      -3.773001     1.230251    -1.374545      52.99
 H      -3.750603     1.398840    -0.280079      25.48
 C      -3.562849     2.330884    -2.214414      21.65
 O      -3.236793     3.514857    -1.737575     243.52
 C      -3.760627     4.011233    -0.436124     102.13
 H      -3.117945     3.626629     0.379587      29.54
 H      -4.792334     3.619965    -0.348235      28.65
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 H      -3.651683     5.085341    -0.508672      26.15
 C      -3.737573     2.239301    -3.637934      21.81
 O      -3.724347     3.300702    -4.562831      90.37
 H      -4.007848     4.166275    -4.255369      21.30
 C      -3.946492     0.912440    -4.119352      57.93
 H      -4.119227     0.669496    -5.185326      25.06
 C      -3.838469    -0.095063    -1.864265      14.81
 C      -3.920165    -1.304773    -0.889029      77.68
 H      -4.564455    -2.038777    -1.408743      24.63
 O      -4.558987    -0.899650     0.325469     174.64
 H      -3.934842    -0.326897     0.868217      25.07
 C      -2.524250    -2.019205    -0.726556      81.68
 H      -2.238809    -2.322561    -1.785771      25.70
 C      -2.576631    -3.403935     0.205110     103.06
 O      -3.221165    -4.528400    -0.441476     246.52
 H      -2.715298    -5.007994    -1.147919      27.12
 H      -3.190943    -3.159572     1.100303      25.64
 H      -1.517035    -3.560894     0.527528      24.94
 C       1.746988    -1.501868    -1.560022      57.55
 H       2.303013    -1.725598    -2.481396      19.16
 C       1.835085    -0.385315     0.658645      59.16
 H       2.485521     0.217663     1.319124      24.17
 C       0.443887    -0.469455     0.781814      12.24
 O      -0.281977     0.023437     1.852114     215.10
 C       0.350830     0.446351     3.066203     114.93
 H      -0.424385     0.577691     3.825216      25.99
 H       1.181240    -0.192048     3.365528      27.80
 H       0.641204     1.479809     2.919903      26.51
 C      -0.298034    -1.180851    -0.249206      12.25
 O      -1.635194    -1.083619    -0.066719     171.22
 C       0.336246    -1.762043    -1.348956      68.53
 H      -0.380648    -2.220994    -2.098858      22.64
 C       2.471769    -0.805981    -0.548165      18.66
 C       4.030078    -0.618366    -0.741387      93.36
 H       4.227431    -0.841853    -1.791515      23.23
 O       4.386708     0.688770    -0.232103     268.07
 H       5.318926     0.735239    -0.536739      20.46
 C       4.921573    -1.647764     0.001878      83.28
 H       4.696495    -1.535793     1.115431      24.54
 O       4.572272    -3.072071    -0.340553     290.40
 H       4.702752    -3.122127    -1.304955      28.91
 C       6.461402    -1.523961    -0.289251      92.91
 O       6.924550    -0.089736    -0.518076     355.43
 H       7.442021     0.090605     0.336287      26.55
 H       6.730364    -2.031602    -1.270353      28.27
 H       7.075212    -2.024965     0.517183      27.18
55
name= lig-ACN-Water-frame_54
 C      -3.958548    -0.217915    -3.234327      54.45
 H      -3.882999    -1.205038    -3.674379      20.44
 C      -3.676377     1.231229    -1.362428      50.52
 H      -3.725095     1.436179    -0.334645      19.50
 C      -3.618355     2.346696    -2.230108      24.81
 O      -3.269967     3.659769    -1.741278     227.17
 C      -3.754078     4.043374    -0.449935     118.02
 H      -3.170348     3.576565     0.409641      26.41
 H      -4.790551     3.742975    -0.213212      25.98
 H      -3.750294     5.069706    -0.428834      27.08
 C      -3.780961     2.223658    -3.633654      12.29
 O      -3.701176     3.335027    -4.425179     -14.06
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 H      -3.983357     4.089575    -3.864200      25.38
 C      -4.007078     0.913775    -4.151123      45.35
 H      -4.178561     0.850892    -5.200581      24.32
 C      -3.873274    -0.059011    -1.875320      30.44
 C      -3.998181    -1.304089    -0.929200      85.13
 H      -4.725826    -2.043398    -1.287826      24.86
 O      -4.606027    -0.910203     0.300443     138.55
 H      -3.940630    -0.348546     0.973719      19.88
 C      -2.599750    -2.108093    -0.680228      87.59
 H      -2.154945    -2.275779    -1.733938      26.02
 C      -2.598407    -3.391592     0.155260     120.11
 O      -3.221249    -4.546325    -0.480285     249.16
 H      -2.472425    -4.958278    -0.909621      29.21
 H      -3.156267    -3.190837     1.079347      26.90
 H      -1.600427    -3.732526     0.465753      25.82
 C       1.766582    -1.472186    -1.547565      44.42
 H       2.310298    -1.782038    -2.464568      20.42
 C       1.870671    -0.337688     0.676326      63.32
 H       2.352075     0.123150     1.478267      25.29
 C       0.481677    -0.501003     0.783826      11.06
 O      -0.318976    -0.001819     1.798553     205.75
 C       0.368237     0.536971     2.982594     120.21
 H      -0.307925     0.347267     3.820739      25.37
 H       1.243393    -0.098825     3.191998      25.97
 H       0.690317     1.509637     2.821596      27.48
 C      -0.253082    -1.183719    -0.237954       0.43
 O      -1.694921    -1.085601    -0.079019     127.12
 C       0.357355    -1.692517    -1.426939      64.36
 H      -0.166510    -2.215001    -2.222185      23.32
 C       2.497680    -0.855889    -0.509622      27.49
 C       3.972398    -0.648506    -0.742043     125.54
 H       4.178412    -0.569028    -1.774739      21.82
 O       4.365873     0.721223    -0.298083     286.36
 H       5.317467     0.766865    -0.425285      18.44
 C       4.927555    -1.662333    -0.040731      84.71
 H       4.783923    -1.540574     1.099067      24.45
 O       4.570169    -3.019332    -0.374384     291.26
 H       4.642798    -3.093153    -1.350259      28.51
 C       6.478882    -1.506641    -0.268813      87.81
 O       6.946805    -0.108891    -0.511680     375.21
 H       7.496198     0.293316     0.340170      25.24
 H       6.803370    -2.238027    -1.111967      27.80
 H       6.931252    -1.824780     0.699113      26.49
55
name= lig-ACN-Water-frame_55
 C      -3.990220    -0.206564    -3.323574      23.10
 H      -4.324382    -1.179012    -3.766361      19.74
 C      -3.633451     1.270980    -1.313631      45.48
 H      -3.407789     1.344004    -0.305080      22.74
 C      -3.623476     2.389385    -2.164503      10.52
 O      -3.340310     3.764068    -1.796786     204.22
 C      -3.767730     4.085552    -0.400377     110.41
 H      -2.967222     3.657555     0.300694      27.24
 H      -4.776590     3.726862    -0.262199      26.81
 H      -3.676076     5.077144    -0.316248      28.13
 C      -3.830776     2.187303    -3.566699      18.64
 O      -3.708784     3.376474    -4.312973     -50.31
 H      -3.807223     4.233791    -3.706165      22.73
 C      -4.013685     0.927425    -4.138866      81.94
 H      -4.215675     0.812238    -5.160848      24.46
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 C      -3.879427    -0.075327    -1.852728     -30.06
 C      -3.984822    -1.317597    -0.946282      77.92
 H      -4.612204    -2.001950    -1.523580      28.31
 O      -4.678365    -0.913853     0.322597     105.58
 H      -3.858429    -0.713060     1.039977      21.75
 C      -2.643376    -2.079531    -0.744463      80.11
 H      -2.311581    -2.521693    -1.771928      27.29
 C      -2.643821    -3.372704     0.160252     110.66
 O      -3.225875    -4.551139    -0.530940     230.50
 H      -2.561123    -5.140539    -1.006840      28.17
 H      -3.159620    -3.212353     1.102939      26.78
 H      -1.573842    -3.450433     0.309184      26.57
 C       1.779368    -1.452181    -1.499576      52.35
 H       2.202247    -1.898706    -2.421501      21.39
 C       1.891144    -0.348204     0.646384      62.97
 H       2.499782     0.118216     1.326871      23.76
 C       0.448271    -0.548964     0.752233       8.64
 O      -0.336109    -0.018954     1.767850     200.88
 C       0.399648     0.575464     2.902080     116.64
 H      -0.339771     0.532719     3.714194      26.12
 H       1.357823     0.072087     3.155617      26.19
 H       0.492828     1.587106     2.752143      28.34
 C      -0.332515    -1.176180    -0.295189      20.90
 O      -1.711139    -1.138353    -0.086294     153.22
 C       0.400270    -1.584147    -1.429663      55.75
 H      -0.071530    -2.013002    -2.248724      24.73
 C       2.541728    -0.865886    -0.474336      28.03
 C       4.004081    -0.590053    -0.780274     105.47
 H       4.082656    -0.788402    -1.797124      23.88
 O       4.341310     0.767751    -0.351142     281.67
 H       5.338071     0.758316    -0.489986      18.66
 C       4.940514    -1.673738    -0.048370      90.28
 H       4.620175    -1.622147     1.061517      24.33
 O       4.564017    -2.989109    -0.400132     303.68
 H       4.792412    -3.109421    -1.395270      27.11
 C       6.495815    -1.446807    -0.204130      90.52
 O       6.952437    -0.139425    -0.517910     339.09
 H       7.666277     0.034440     0.308982      24.65
 H       6.881010    -2.060014    -1.126646      27.25
 H       7.018763    -1.862968     0.683845      27.20
55
name= lig-ACN-Water-frame_56
 C      -4.086334    -0.187917    -3.258184      53.11
 H      -4.403457    -1.190347    -3.703234      24.76
 C      -3.596639     1.227562    -1.288253      65.20
 H      -3.333697     1.264195    -0.253454      26.71
 C      -3.596234     2.418443    -2.077152       8.99
 O      -3.460898     3.759194    -1.806130     239.66
 C      -3.722745     4.136349    -0.395111     117.20
 H      -3.019584     3.591720     0.319408      28.26
 H      -4.661806     3.707771    -0.093378      28.16
 H      -3.778196     5.152305    -0.342090      27.94
 C      -3.819416     2.304877    -3.484840      -5.72
 O      -3.738068     3.368012    -4.272045      -8.16
 H      -4.024462     4.301315    -3.809595      19.73
 C      -4.003600     0.986766    -4.111087      40.63
 H      -4.221554     0.948290    -5.174256      26.08
 C      -3.839437    -0.024270    -1.922438      43.68
 C      -3.990282    -1.272890    -0.951942      56.79
 H      -4.702663    -2.015874    -1.329184      24.11
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 O      -4.679681    -0.967967     0.297062     117.11
 H      -4.066727    -0.477448     0.995158      24.19
 C      -2.656814    -2.066418    -0.795831      91.43
 H      -2.291131    -2.184506    -1.892230      25.67
 C      -2.655404    -3.371997     0.088957     114.18
 O      -3.255885    -4.522251    -0.559209     259.27
 H      -2.444042    -4.905398    -1.049969      27.54
 H      -3.230055    -3.198232     1.012098      26.26
 H      -1.683203    -3.677496     0.444406      25.67
 C       1.810393    -1.478407    -1.511817      46.11
 H       2.430883    -1.716649    -2.393042      16.13
 C       1.805849    -0.402198     0.633440      66.83
 H       2.196232     0.259805     1.364058      24.75
 C       0.434204    -0.538147     0.716866      18.91
 O      -0.296198    -0.043074     1.781671     220.25
 C       0.349786     0.649546     2.845920     122.86
 H      -0.237065     0.586244     3.766990      26.64
 H       1.324053     0.147898     3.082144      26.30
 H       0.568168     1.613046     2.504653      28.41
 C      -0.348697    -1.123490    -0.312598      25.28
 O      -1.722965    -1.196520    -0.124418     170.17
 C       0.330077    -1.542477    -1.450023      64.61
 H      -0.220095    -1.866122    -2.266764      25.49
 C       2.571158    -0.827823    -0.519304      18.50
 C       4.081749    -0.607683    -0.787428     100.39
 H       4.331598    -0.626591    -1.781146      22.53
 O       4.347792     0.794232    -0.426617     299.38
 H       5.358298     0.949409    -0.565464      18.29
 C       4.936551    -1.590069     0.002301      82.93
 H       4.718480    -1.494047     1.123431      23.93
 O       4.571651    -3.004031    -0.426811     295.37
 H       4.825112    -3.129172    -1.452826      26.68
 C       6.492075    -1.516962    -0.197421      83.78
 O       6.975490    -0.096009    -0.510553     332.68
 H       7.533745     0.253882     0.342962      25.00
 H       6.688936    -2.213750    -1.101495      29.53
 H       7.022639    -1.888827     0.686413      28.22
55
name= lig-ACN-Water-frame_57
 C      -4.154504    -0.066390    -3.254532      42.75
 H      -4.259015    -1.079536    -3.766970      32.23
 C      -3.533995     1.242524    -1.280346      54.43
 H      -3.485493     1.346785    -0.165310      23.23
 C      -3.604375     2.391018    -2.079144       8.23
 O      -3.558748     3.745312    -1.688658     232.12
 C      -3.710416     4.135364    -0.372631     126.13
 H      -2.790874     3.903475     0.216822      28.14
 H      -4.637858     3.855064     0.062065      27.93
 H      -3.642552     5.211819    -0.416975      26.86
 C      -3.784983     2.270663    -3.454746      17.21
 O      -3.787764     3.410070    -4.338998      67.86
 H      -4.080648     4.308478    -3.859951      20.78
 C      -4.016543     1.076046    -4.011375      67.22
 H      -4.198462     1.122227    -5.116506      23.16
 C      -3.844360    -0.040499    -1.829801     -28.48
 C      -4.012076    -1.256892    -0.980365      78.35
 H      -4.674125    -1.895806    -1.579932      21.29
 O      -4.631429    -0.984104     0.298814     126.34
 H      -4.176986    -0.317944     0.709591      31.26
 C      -2.597657    -2.071812    -0.844315      84.56
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 H      -2.246291    -2.378111    -1.894495      26.33
 C      -2.688994    -3.356945     0.005756     111.40
 O      -3.285608    -4.500950    -0.621960     238.51
 H      -2.679300    -5.001743    -1.183981      29.29
 H      -3.376435    -3.059023     0.828302      25.08
 H      -1.683425    -3.521644     0.348434      26.33
 C       1.747872    -1.442869    -1.596447      58.97
 H       2.054464    -1.833126    -2.568034      19.49
 C       1.828966    -0.375995     0.588361      51.76
 H       2.432162     0.110596     1.410169      23.06
 C       0.392200    -0.504819     0.714969       5.76
 O      -0.332810    -0.091249     1.815319     192.84
 C       0.370254     0.723431     2.822106     112.62
 H      -0.431810     0.812573     3.563534      26.11
 H       1.274933     0.226709     3.232474      26.69
 H       0.542783     1.767033     2.537092      27.89
 C      -0.342557    -1.121670    -0.358854      10.50
 O      -1.721194    -1.156219    -0.106013     149.06
 C       0.378713    -1.556301    -1.524516      65.14
 H      -0.109651    -2.009611    -2.373470      25.47
 C       2.526143    -0.813054    -0.577009      15.52
 C       4.077564    -0.574562    -0.774085      96.89
 H       4.226772    -0.849875    -1.762561      24.68
 O       4.374748     0.814775    -0.464647     293.09
 H       5.347370     0.887947    -0.665732      20.22
 C       4.974400    -1.653087     0.018385      88.60
 H       4.664836    -1.591025     1.103518      24.95
 O       4.589502    -2.947855    -0.352613     323.91
 H       4.772257    -3.106069    -1.382196      26.08
 C       6.483296    -1.494215    -0.238802     101.66
 O       6.975461    -0.105664    -0.502357     356.13
 H       7.495398     0.130453     0.361761      27.16
 H       6.854299    -2.065923    -1.145156      28.99
 H       7.004536    -1.894772     0.633224      27.87
55
name= lig-ACN-Water-frame_58
 C      -4.110071    -0.043255    -3.175290      58.53
 H      -4.461363    -0.975832    -3.679574      21.45
 C      -3.543845     1.274054    -1.238623      60.65
 H      -3.363792     1.471434    -0.114492      18.15
 C      -3.612570     2.433580    -2.048753      22.32
 O      -3.627033     3.699074    -1.636163     225.21
 C      -3.664977     4.211369    -0.222721     109.47
 H      -2.847608     3.801428     0.329263      28.13
 H      -4.503482     3.803972     0.303595      26.34
 H      -3.778097     5.328791    -0.377928      24.16
 C      -3.758308     2.420497    -3.520028      24.52
 O      -3.836731     3.398012    -4.385098     142.57
 H      -3.926872     4.311088    -3.978242      21.98
 C      -4.058893     1.101263    -4.035240      31.58
 H      -4.241145     0.864530    -5.146542      22.82
 C      -3.887624     0.026629    -1.821498      49.80
 C      -3.936074    -1.317670    -1.041143      92.69
 H      -4.667665    -2.047954    -1.430605      26.89
 O      -4.595194    -1.013343     0.274464     143.47
 H      -4.018265    -0.502594     0.919050      23.83
 C      -2.610776    -2.035184    -0.898740      96.30
 H      -2.138784    -2.199581    -1.895459      26.83
 C      -2.724588    -3.321206    -0.026457     110.18
 O      -3.346766    -4.501798    -0.721643     233.08
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 H      -2.569249    -4.925923    -1.127652      29.18
 H      -3.288707    -3.208541     0.940642      25.40
 H      -1.752824    -3.644517     0.315140      25.92
 C       1.751645    -1.366897    -1.702155      43.22
 H       2.421373    -1.738345    -2.471173      20.19
 C       1.834643    -0.338966     0.522133      46.94
 H       2.533637    -0.044972     1.405640      22.52
 C       0.455647    -0.486567     0.676125       7.04
 O      -0.341684    -0.118289     1.841023     166.60
 C       0.294329     0.770290     2.842556     109.69
 H      -0.414532     1.019680     3.640271      25.66
 H       1.177425     0.309836     3.323906      25.43
 H       0.648878     1.630962     2.183056      26.29
 C      -0.327460    -1.107388    -0.376558      13.83
 O      -1.704577    -1.113146    -0.125798     141.75
 C       0.308709    -1.588316    -1.527205      70.28
 H      -0.273387    -2.161462    -2.311641      23.57
 C       2.486240    -0.800355    -0.644824      22.50
 C       3.986299    -0.619150    -0.778112      95.54
 H       4.235708    -0.684218    -1.792555      22.15
 O       4.410962     0.784831    -0.487313     284.43
 H       5.356561     0.810837    -0.620464      19.37
 C       4.958067    -1.605250     0.011329      88.95
 H       4.890817    -1.478513     1.106678      24.14
 O       4.585117    -2.977417    -0.274279     296.58
 H       4.842294    -3.197467    -1.260921      26.52
 C       6.542774    -1.442724    -0.280261      94.34
 O       6.961943    -0.123514    -0.493567     386.39
 H       7.434252     0.178048     0.325258      28.12
 H       6.671879    -2.026304    -1.217511      29.33
 H       7.112582    -1.948274     0.505157      27.93
55
name= lig-ACN-Water-frame_59
 C      -4.093679    -0.027628    -3.194647      59.37
 H      -4.424641    -0.981494    -3.561261      22.60
 C      -3.608996     1.326713    -1.235857      43.14
 H      -3.338548     1.369209    -0.115751      21.38
 C      -3.633634     2.477139    -2.073417      10.85
 O      -3.660713     3.823805    -1.532232     181.45
 C      -3.650430     4.166635    -0.133133     110.95
 H      -2.727112     3.964800     0.276917      30.61
 H      -4.518419     3.808825     0.400759      27.62
 H      -3.653342     5.361931    -0.117939      24.33
 C      -3.807668     2.311916    -3.508833      12.05
 O      -3.845173     3.460586    -4.474630     -23.47
 H      -4.260087     4.254398    -4.027385      20.85
 C      -4.050241     1.077086    -4.037900      62.80
 H      -4.355907     1.132923    -5.137955      29.28
 C      -3.869880     0.045810    -1.801540      14.39
 C      -3.938273    -1.248275    -1.000890      79.34
 H      -4.507584    -1.953953    -1.643973      26.07
 O      -4.566102    -1.086214     0.254217     129.50
 H      -3.808282    -0.904163     1.022880      21.33
 C      -2.566208    -1.999431    -0.870248      91.09
 H      -2.284049    -2.234769    -1.892215      28.06
 C      -2.725813    -3.386999    -0.058983     107.57
 O      -3.366513    -4.444929    -0.808652     190.33
 H      -2.651863    -5.013907    -1.268485      27.09
 H      -3.361349    -3.038919     0.804793      25.68
 H      -1.703332    -3.670650     0.206183      24.98
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 C       1.705260    -1.349898    -1.726418      45.60
 H       2.073745    -1.678084    -2.691499      21.90
 C       1.826572    -0.334513     0.518021      52.69
 H       2.373201     0.209830     1.399787      20.49
 C       0.420925    -0.461886     0.705795      17.47
 O      -0.293670    -0.157214     1.822256     211.35
 C       0.249048     0.780069     2.786072     116.80
 H      -0.609128     1.137872     3.376894      24.66
 H       0.992377     0.249198     3.393580      24.27
 H       0.753505     1.764418     2.357035      24.75
 C      -0.314335    -1.071837    -0.362725      15.86
 O      -1.695131    -1.098167    -0.169773     177.25
 C       0.339583    -1.594642    -1.533722      60.29
 H      -0.298052    -2.118651    -2.356786      19.54
 C       2.477904    -0.739940    -0.694310      41.40
 C       4.022822    -0.634848    -0.855042     102.51
 H       4.206927    -0.886757    -1.889109      20.91
 O       4.413463     0.747856    -0.466483     270.15
 H       5.411979     0.709411    -0.564699      15.87
 C       4.951421    -1.557393     0.015802      84.30
 H       4.665609    -1.311353     1.026853      24.09
 O       4.600188    -3.027719    -0.192674     319.67
 H       4.744013    -3.144743    -1.166515      27.15
 C       6.479523    -1.497140    -0.372777     106.75
 O       6.988621    -0.052298    -0.497244     395.35
 H       7.355284     0.297852     0.379304      29.00
 H       6.705169    -1.937919    -1.322719      30.19
 H       7.046486    -1.989748     0.419733      27.94
55
name= lig-ACN-Water-frame_60
 C      -4.101036    -0.097578    -3.232591      49.64
 H      -4.168118    -1.039635    -3.707323      29.03
 C      -3.665068     1.390420    -1.269998      59.39
 H      -3.631927     1.522172    -0.161400      20.81
 C      -3.695760     2.605308    -2.031764      16.24
 O      -3.674940     3.893569    -1.547017     225.41
 C      -3.616421     4.099503    -0.081119     108.73
 H      -2.765000     3.631854     0.309909      29.30
 H      -4.415598     3.584722     0.494536      27.57
 H      -3.731383     5.298979    -0.058335      24.06
 C      -3.864801     2.459981    -3.492973      11.68
 O      -3.851395     3.382660    -4.455895      74.97
 H      -4.019024     4.307793    -4.130264      20.22
 C      -4.036672     1.068743    -4.044345      26.37
 H      -4.233674     0.900301    -5.138265      22.46
 C      -3.817541     0.090777    -1.815790      29.00
 C      -3.908088    -1.213076    -1.004555      72.32
 H      -4.673232    -1.832390    -1.521729      21.98
 O      -4.572615    -1.174550     0.314238     148.75
 H      -3.920490    -0.726456     1.003585      23.13
 C      -2.557377    -2.027735    -0.884369      95.17
 H      -2.137836    -2.228180    -1.838336      26.80
 C      -2.679187    -3.362337    -0.110713     113.33
 O      -3.375246    -4.370424    -0.896390     234.33
 H      -2.673891    -4.909720    -1.379618      28.11
 H      -3.282080    -3.414045     0.831992      24.69
 H      -1.707973    -3.748895     0.282802      24.91
 C       1.704280    -1.356564    -1.682796      35.34
 H       2.192258    -1.675687    -2.604925      17.02
 C       1.824871    -0.306539     0.499915      59.25
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 H       2.495199     0.267573     1.208412      19.33
 C       0.440888    -0.490163     0.650219      18.39
 O      -0.284251    -0.157058     1.799305     209.71
 C       0.223912     0.778199     2.779346     113.88
 H      -0.706838     1.168262     3.254959      24.70
 H       0.796201     0.328726     3.597319      25.40
 H       0.803900     1.634973     2.192956      23.91
 C      -0.329119    -1.096847    -0.378401      30.05
 O      -1.682562    -1.090064    -0.184259     180.96
 C       0.316248    -1.529916    -1.488948      68.94
 H      -0.246251    -1.978094    -2.388198      21.24
 C       2.491712    -0.721409    -0.709848      40.96
 C       4.028044    -0.611320    -0.922594     107.30
 H       4.324324    -0.702579    -1.989102      20.13
 O       4.431411     0.718596    -0.475283     285.44
 H       5.468314     0.764554    -0.578754      16.97
 C       4.894113    -1.634827    -0.048280      88.18
 H       4.855791    -1.397002     0.985431      25.66
 O       4.641109    -2.993591    -0.117140     325.82
 H       4.596199    -3.231793    -1.040003      31.31
 C       6.411157    -1.422998    -0.417989     105.84
 O       6.984790    -0.025161    -0.504290     323.59
 H       7.511575     0.026079     0.404545      26.31
 H       6.518233    -1.819299    -1.376182      31.79
 H       7.013819    -2.036816     0.270936      29.33
55
name= lig-ACN-Water-frame_61
 C      -3.994402    -0.034314    -3.206618      77.16
 H      -4.098081    -1.000133    -3.647331      29.00
 C      -3.743500     1.457378    -1.294870      46.06
 H      -3.730051     1.511475    -0.235767      24.00
 C      -3.798056     2.625717    -2.095499      23.42
 O      -3.677616     3.936689    -1.559738     172.89
 C      -3.596394     3.980427    -0.096979     114.51
 H      -2.653201     3.596336     0.276806      26.57
 H      -4.555254     3.534567     0.304498      24.92
 H      -3.547428     5.108359     0.165894      24.29
 C      -3.916884     2.378788    -3.462233      20.38
 O      -3.847235     3.392102    -4.456053      21.80
 H      -3.903723     4.252864    -4.041267      21.30
 C      -4.014538     1.138376    -3.971425      95.29
 H      -3.984685     1.155661    -5.047502      28.78
 C      -3.835893     0.106142    -1.857488     -23.78
 C      -3.914148    -1.261355    -0.981354      42.67
 H      -4.548277    -1.969712    -1.573670      22.56
 O      -4.552829    -1.200854     0.388226     124.35
 H      -4.239845    -0.509821     0.896762      29.49
 C      -2.566846    -2.016315    -0.905537      88.86
 H      -2.271794    -2.215201    -1.891724      28.26
 C      -2.650872    -3.364080    -0.100501     112.07
 O      -3.353487    -4.303949    -1.016545     193.90
 H      -2.614405    -4.781521    -1.418062      29.52
 H      -3.152594    -3.010259     0.820548      25.17
 H      -1.588324    -3.711936    -0.044438      24.76
 C       1.751245    -1.378649    -1.669882      40.51
 H       2.279639    -1.835206    -2.516558      22.18
 C       1.877585    -0.249063     0.447209      60.73
 H       2.346621     0.151494     1.318951      24.38
 C       0.494706    -0.497318     0.672651       8.96
 O      -0.299868    -0.163473     1.764620     202.52
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 C       0.194980     0.795290     2.783891     115.05
 H      -0.620698     1.413015     3.240341      25.49
 H       0.799180     0.210934     3.494004      23.94
 H       0.938056     1.557069     2.308095      24.80
 C      -0.333928    -1.102270    -0.350663       7.81
 O      -1.714245    -1.092962    -0.149991     146.80
 C       0.317748    -1.507091    -1.577529      59.29
 H      -0.292229    -1.970107    -2.381009      24.71
 C       2.527522    -0.733621    -0.697643      42.57
 C       3.989275    -0.593156    -0.896653     104.66
 H       4.141126    -0.730883    -2.018691      20.24
 O       4.438517     0.743526    -0.497492     278.07
 H       5.487325     0.740206    -0.604579      13.22
 C       4.909907    -1.537962    -0.072578      85.05
 H       4.629792    -1.227384     0.898374      25.72
 O       4.644053    -3.025842    -0.100018     316.63
 H       4.765086    -3.277706    -1.065076      27.97
 C       6.409420    -1.362177    -0.509789     107.11
 O       6.961695    -0.061992    -0.492580     357.31
 H       7.440375     0.324576     0.392476      25.32
 H       6.503106    -1.678100    -1.504534      30.74
 H       7.010802    -2.017398     0.135613      28.28
55
name= lig-ACN-Water-frame_62
 C      -3.882018    -0.000059    -3.205021      22.02
 H      -4.007904    -0.978782    -3.719812      20.74
 C      -3.847531     1.403334    -1.252955      69.97
 H      -3.642780     1.557160    -0.256285      25.09
 C      -3.865528     2.593170    -2.059297      11.67
 O      -3.675364     3.893778    -1.591949     219.58
 C      -3.587933     3.904164    -0.161042     108.77
 H      -2.760390     3.230602     0.212346      26.96
 H      -4.493266     3.493428     0.434564      24.47
 H      -3.492883     4.977750     0.053103      25.74
 C      -3.925947     2.473011    -3.503797      16.47
 O      -3.834072     3.443478    -4.423715     -45.52
 H      -4.202391     4.307257    -4.138217      23.45
 C      -3.972049     1.124875    -4.044354      42.19
 H      -4.118755     1.005743    -5.091528      28.57
 C      -3.908880     0.089935    -1.716149      -6.89
 C      -3.959976    -1.246807    -0.936133      90.90
 H      -4.673605    -1.906300    -1.484626      26.38
 O      -4.544246    -1.188607     0.361069     171.69
 H      -4.002556    -0.599006     0.946376      25.51
 C      -2.565617    -1.946324    -0.887758     104.90
 H      -2.196676    -2.063532    -1.866836      30.34
 C      -2.614281    -3.305679    -0.209999     115.36
 O      -3.326269    -4.231344    -1.068462     236.91
 H      -2.661449    -4.828361    -1.486017      29.02
 H      -3.169739    -3.490125     0.716195      26.34
 H      -1.603771    -3.680031     0.140291      26.61
 C       1.740214    -1.427131    -1.699062      52.45
 H       2.158847    -1.840106    -2.631799      21.04
 C       1.851588    -0.223157     0.523901      58.66
 H       2.495596     0.250273     1.161761      24.51
 C       0.448293    -0.487507     0.669002       9.90
 O      -0.309358    -0.110792     1.766113     183.80
 C       0.259751     0.778283     2.757998     110.44
 H      -0.713240     1.229515     3.125948      25.84
 H       0.620368     0.208929     3.646074      25.99
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 H       0.950913     1.530132     2.345961      27.92
 C      -0.279547    -1.090521    -0.416422      15.75
 O      -1.681930    -1.101168    -0.116484     161.28
 C       0.354328    -1.503813    -1.582312      82.10
 H      -0.141557    -1.963487    -2.387310      28.31
 C       2.484964    -0.755576    -0.675241      -3.64
 C       4.015802    -0.574670    -0.906373     103.53
 H       4.270585    -0.805437    -2.022093      19.79
 O       4.397308     0.801792    -0.536770     283.72
 H       5.404033     0.830660    -0.605463      16.03
 C       4.933213    -1.508522    -0.057622      94.33
 H       4.968099    -1.273411     0.980485      25.12
 O       4.655366    -2.967184    -0.131451     305.68
 H       4.829866    -3.218093    -1.134907      26.56
 C       6.423661    -1.398260    -0.547160     100.58
 O       6.959837     0.007149    -0.500736     353.93
 H       7.312076     0.097002     0.497724      26.27
 H       6.470581    -1.647816    -1.590523      30.87
 H       7.033345    -2.128562     0.003863      29.97
55
name= lig-ACN-Water-frame_63
 C      -3.868826    -0.006365    -3.141943      60.22
 H      -3.766601    -1.051185    -3.589880      26.74
 C      -3.935815     1.389390    -1.158231      59.51
 H      -3.946176     1.479817    -0.103026      24.39
 C      -3.880433     2.495197    -2.093171       1.06
 O      -3.700851     3.773800    -1.606330     178.29
 C      -3.568065     3.899753    -0.160423     107.17
 H      -2.680805     3.235685     0.204402      28.11
 H      -4.613187     3.617501     0.251450      25.01
 H      -3.295709     4.867072     0.087136      27.96
 C      -3.919507     2.426549    -3.530780     -10.08
 O      -3.841373     3.569311    -4.411906     -72.29
 H      -4.015646     4.438785    -3.896032      23.30
 C      -3.911277     1.124871    -4.048687      41.08
 H      -4.112133     0.912726    -5.071365      23.05
 C      -3.965717     0.090064    -1.793586      17.49
 C      -3.972724    -1.204187    -0.938704      69.57
 H      -4.577289    -1.960607    -1.485934      26.01
 O      -4.571315    -1.128688     0.375579     144.12
 H      -3.881561    -0.917828     1.196408      21.92
 C      -2.552948    -1.879568    -0.879689      90.15
 H      -2.236389    -1.962913    -1.910998      29.79
 C      -2.619498    -3.322273    -0.246666     119.85
 O      -3.307594    -4.213091    -1.148567     222.68
 H      -2.528170    -4.733148    -1.590135      26.89
 H      -3.132349    -3.057330     0.670470      27.35
 H      -1.551990    -3.643627    -0.159392      25.48
 C       1.770550    -1.408305    -1.675442      51.89
 H       2.387014    -1.653634    -2.558240      20.60
 C       1.826574    -0.299466     0.488936      86.46
 H       2.239617     0.299202     1.211248      29.95
 C       0.462335    -0.431231     0.656561       3.69
 O      -0.311676    -0.068407     1.733369     205.69
 C       0.253029     0.766278     2.791478     115.23
 H      -0.517383     1.454931     3.242914      25.70
 H       0.855853     0.149604     3.517083      24.65
 H       0.991002     1.397540     2.359495      27.31
 C      -0.297905    -1.040387    -0.395526       6.36
 O      -1.609722    -1.082682    -0.096068     173.19
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 C       0.327993    -1.560983    -1.575948      79.11
 H      -0.259347    -1.959936    -2.321190      27.93
 C       2.493761    -0.766311    -0.671941      30.38
 C       4.008543    -0.559775    -0.848110     100.61
 H       4.262075    -0.662189    -1.999667      19.72
 O       4.321685     0.867776    -0.601675     318.38
 H       5.276874     0.878213    -0.526988      18.02
 C       5.040859    -1.550519    -0.042813      82.42
 H       4.889277    -1.257178     1.000397      25.97
 O       4.648772    -2.866614    -0.176330     357.88
 H       4.692067    -3.090715    -1.209476      25.98
 C       6.457868    -1.362400    -0.586578     103.60
 O       6.939163     0.022271    -0.489666     367.95
 H       7.498602     0.241364     0.307428      28.51
 H       6.489523    -1.626577    -1.673395      30.51
 H       7.153529    -1.993491    -0.026064      28.42
55
name= lig-ACN-Water-frame_64
 C      -3.891670    -0.029382    -3.207421      62.47
 H      -3.804802    -1.085604    -3.680210      21.63
 C      -4.045873     1.362658    -1.226985      86.50
 H      -4.308482     1.488883    -0.154302      23.82
 C      -3.864716     2.448791    -2.073070       9.96
 O      -3.720023     3.713025    -1.595415     173.59
 C      -3.559263     3.916598    -0.176971     114.37
 H      -2.779876     3.193101     0.357365      26.63
 H      -4.489148     3.799268     0.506241      26.03
 H      -3.317417     4.903660    -0.166632      27.86
 C      -3.881219     2.396024    -3.521369      -5.31
 O      -3.840556     3.535259    -4.338877     -34.61
 H      -4.134460     4.464980    -3.915105      19.07
 C      -3.875068     1.080644    -4.049029      50.31
 H      -3.721129     1.019707    -5.130407      23.02
 C      -3.990470     0.099437    -1.747727     -11.78
 C      -3.924494    -1.187612    -0.938104      69.02
 H      -4.543715    -1.933117    -1.464830      22.79
 O      -4.636660    -1.077552     0.408445     134.21
 H      -3.906331    -0.583497     1.072974      21.86
 C      -2.535327    -1.849195    -0.925592      93.89
 H      -2.178669    -1.908351    -1.987204      26.26
 C      -2.606468    -3.243073    -0.291145     116.21
 O      -3.318873    -4.202110    -1.213350     223.53
 H      -2.591363    -4.787732    -1.602326      26.82
 H      -3.098100    -3.426505     0.647720      25.86
 H      -1.607804    -3.653057    -0.042551      24.86
 C       1.750642    -1.379437    -1.664394      69.72
 H       2.121426    -1.793152    -2.618749      22.00
 C       1.863698    -0.307162     0.506737      44.52
 H       2.546600     0.033498     1.275079      20.19
 C       0.448089    -0.406489     0.619710      16.24
 O      -0.335250     0.003494     1.729227     201.03
 C       0.334489     0.771523     2.790584     112.98
 H      -0.530482     1.213277     3.341055      24.94
 H       0.740292     0.016988     3.521094      24.60
 H       0.999622     1.493076     2.448054      27.80
 C      -0.280555    -1.046541    -0.401785      15.35
 O      -1.670875    -1.059028    -0.086722     163.78
 C       0.365769    -1.574805    -1.522636      65.95
 H      -0.151854    -2.069954    -2.300196      21.52
 C       2.552004    -0.778616    -0.637756      30.66
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 C       4.029126    -0.521525    -0.824423      90.90
 H       4.176844    -0.872816    -1.951895      15.76
 O       4.265267     0.924664    -0.619044     272.40
 H       5.237115     0.965291    -0.677571      20.30
 C       5.041982    -1.425497    -0.053987      88.99
 H       5.075957    -1.251840     1.055671      23.34
 O       4.609381    -2.864825    -0.224262     330.76
 H       4.810002    -3.047840    -1.225820      25.62
 C       6.552606    -1.295221    -0.574292      95.82
 O       6.915452     0.071544    -0.501983     425.06
 H       7.266938     0.160928     0.379092      32.24
 H       6.561615    -1.589417    -1.690427      30.50
 H       7.220906    -2.008181    -0.065411      28.98
55
name= lig-ACN-Water-frame_65
 C      -3.911519    -0.084235    -3.225350      63.08
 H      -3.937932    -1.112810    -3.725020      26.96
 C      -4.158255     1.334218    -1.292277      64.69
 H      -4.263069     1.562655    -0.167291      22.67
 C      -3.894307     2.479607    -2.062787      21.99
 O      -3.747296     3.746476    -1.550605     205.25
 C      -3.559556     3.990988    -0.154800     114.43
 H      -2.705701     3.250430     0.241953      25.87
 H      -4.559029     3.863980     0.348018      27.18
 H      -3.218956     4.977609    -0.019074      26.77
 C      -3.832450     2.365642    -3.466492      11.38
 O      -3.824356     3.405843    -4.278875      80.59
 H      -4.156974     4.329802    -3.856994      19.72
 C      -3.817185     1.092464    -4.071643      62.87
 H      -3.754949     0.932236    -5.200243      24.21
 C      -4.007995     0.014670    -1.844669       6.61
 C      -4.011611    -1.197666    -0.899212      79.69
 H      -4.650401    -1.966712    -1.360830      24.42
 O      -4.628573    -1.027948     0.361270     189.67
 H      -4.158660    -0.407275     0.987788      25.03
 C      -2.568640    -1.853444    -0.899952      83.08
 H      -2.170865    -1.903061    -1.981564      25.54
 C      -2.616107    -3.303912    -0.347672     124.72
 O      -3.328613    -4.153430    -1.254412     258.15
 H      -2.680231    -4.783778    -1.578620      28.97
 H      -3.188445    -3.082135     0.537194      26.94
 H      -1.587908    -3.591865    -0.177938      26.14
 C       1.776209    -1.376176    -1.652019      35.17
 H       2.354781    -1.759367    -2.502452      23.45
 C       1.901984    -0.316899     0.572089      38.03
 H       2.445558     0.047260     1.512490      22.03
 C       0.478348    -0.381624     0.664488       2.32
 O      -0.299776     0.108430     1.689505     212.26
 C       0.363507     0.726448     2.826141     121.72
 H      -0.437963     1.188820     3.410768      25.51
 H       1.032660     0.057805     3.416967      24.88
 H       0.997446     1.493338     2.488439      27.17
 C      -0.344614    -1.043589    -0.350910       7.05
 O      -1.686863    -1.020938    -0.124284     166.09
 C       0.369924    -1.564935    -1.472184      73.36
 H      -0.129867    -2.192050    -2.245624      22.95
 C       2.527610    -0.795491    -0.635316      31.58
 C       4.054550    -0.505333    -0.872633      93.59
 H       4.396738    -0.550436    -2.007470      16.27
 O       4.256455     0.942426    -0.623951     279.15
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 H       5.163120     1.178560    -1.042201      19.21
 C       5.054799    -1.439677    -0.075959      76.63
 H       4.973303    -1.163838     1.042405      23.31
 O       4.614536    -2.796248    -0.235524     347.75
 H       4.703297    -3.010902    -1.215887      26.69
 C       6.498477    -1.269529    -0.570143      96.74
 O       6.924793     0.175239    -0.484154     356.64
 H       7.383303     0.439033     0.298969      28.95
 H       6.615622    -1.574100    -1.689164      28.69
 H       7.175393    -1.856203     0.075521      27.25
55
name= lig-ACN-Water-frame_66
 C      -3.917433    -0.137165    -3.292489      54.62
 H      -3.897209    -1.113241    -3.776724      23.48
 C      -4.172138     1.286803    -1.289020      71.83
 H      -4.244421     1.180724    -0.147159      24.94
 C      -3.949565     2.475517    -2.012546      10.56
 O      -3.782789     3.850448    -1.559507     193.36
 C      -3.575693     4.033833    -0.103512     111.94
 H      -2.819057     3.288395     0.401985      26.39
 H      -4.488431     3.902107     0.505657      27.20
 H      -3.277513     5.106588    -0.033724      26.44
 C      -3.802592     2.277025    -3.428118      -4.60
 O      -3.798600     3.401107    -4.315804      92.88
 H      -3.785960     4.233794    -3.750052      24.51
 C      -3.778821     1.010545    -4.026388      58.59
 H      -4.029088     1.115875    -5.145351      27.68
 C      -4.106472     0.021408    -1.893978       9.68
 C      -4.085664    -1.257340    -0.983209      68.48
 H      -4.678475    -2.060117    -1.433003      24.73
 O      -4.640318    -0.968292     0.343373     171.03
 H      -3.964987    -0.596592     0.853426      28.52
 C      -2.626415    -1.866104    -0.930016      78.06
 H      -2.396532    -1.862406    -2.077446      26.23
 C      -2.636730    -3.280604    -0.328418     124.22
 O      -3.366360    -4.139614    -1.294132     215.27
 H      -2.655842    -4.697213    -1.708019      28.12
 H      -3.107658    -3.447565     0.626972      27.41
 H      -1.697473    -3.768772    -0.178555      26.57
 C       1.783824    -1.393712    -1.582056      41.61
 H       2.204729    -1.745754    -2.528006      19.53
 C       1.879477    -0.366013     0.591833      49.93
 H       2.493971     0.277758     1.362916      21.95
 C       0.488629    -0.397395     0.690249      12.27
 O      -0.256682     0.220325     1.689754     209.77
 C       0.426234     0.731828     2.860296     118.51
 H      -0.296551     0.972961     3.608014      27.17
 H       1.002992    -0.105443     3.265317      26.97
 H       0.997339     1.615401     2.598384      26.21
 C      -0.267089    -1.018660    -0.328555       5.87
 O      -1.698698    -0.979068    -0.144899     129.68
 C       0.351267    -1.576314    -1.446174      66.70
 H      -0.339015    -2.103807    -2.209962      24.77
 C       2.585935    -0.729467    -0.595638       3.21
 C       4.037518    -0.460143    -0.922171     104.58
 H       4.057178    -0.780195    -2.057553      21.33
 O       4.254181     0.967223    -0.630007     265.57
 H       5.164901     1.202121    -0.981803      22.81
 C       5.012343    -1.393383    -0.115981      88.30
 H       4.853697    -1.137032     1.010793      24.44
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 O       4.644542    -2.759084    -0.227296     316.35
 H       4.624334    -2.996797    -1.169904      30.20
 C       6.491280    -1.148377    -0.504400      96.49
 O       6.904082     0.230727    -0.499360     291.49
 H       7.258004     0.279913     0.368423      26.57
 H       6.603226    -1.554851    -1.579332      28.83
 H       7.160659    -1.812061     0.097938      28.80
55
name= lig-ACN-Water-frame_67
 C      -3.948485    -0.197844    -3.295249      54.59
 H      -3.962018    -1.149260    -3.723687      21.80
 C      -4.129929     1.269591    -1.228955      35.79
 H      -4.378573     1.418229    -0.151859      18.08
 C      -3.952545     2.494366    -1.988384       5.80
 O      -3.833912     3.821431    -1.548549     213.00
 C      -3.637253     4.069117    -0.074613     107.43
 H      -2.792882     3.388548     0.270464      24.00
 H      -4.555335     3.926792     0.444800      24.87
 H      -3.294301     5.188734     0.013831      23.65
 C      -3.800672     2.354890    -3.437747      12.13
 O      -3.740585     3.360269    -4.309585     135.71
 H      -3.910347     4.251559    -4.019208      21.64
 C      -3.820677     1.027112    -4.062060      34.66
 H      -3.688529     0.891934    -5.195902      28.23
 C      -4.185191    -0.045547    -1.901871      24.51
 C      -4.104113    -1.242277    -1.038092      85.84
 H      -4.757370    -2.024572    -1.416419      27.97
 O      -4.655492    -0.957163     0.303668     180.23
 H      -4.028281    -0.594351     0.899075      26.07
 C      -2.657089    -1.858068    -0.938077      76.81
 H      -2.105060    -2.086976    -1.929299      26.28
 C      -2.662249    -3.322083    -0.326636     115.17
 O      -3.404082    -4.152389    -1.324361     229.05
 H      -2.703568    -4.673993    -1.856339      28.86
 H      -3.212768    -3.304236     0.601542      27.77
 H      -1.620954    -3.504897    -0.218989      28.10
 C       1.742599    -1.421293    -1.548180      31.80
 H       2.232959    -1.762006    -2.453383      20.49
 C       1.916637    -0.307603     0.597203      29.83
 H       2.527374     0.298781     1.387552      23.39
 C       0.477561    -0.389013     0.726268     -24.98
 O      -0.243010     0.316181     1.692780     204.71
 C       0.509824     0.710172     2.916039     114.11
 H      -0.299525     0.817678     3.589121      26.26
 H       1.219529    -0.004370     3.265355      26.81
 H       1.050538     1.685353     2.815061      25.60
 C      -0.335914    -1.030673    -0.318294       4.76
 O      -1.704883    -0.954777    -0.189837     149.82
 C       0.393991    -1.563459    -1.400778      71.57
 H      -0.088698    -2.017680    -2.358354      23.94
 C       2.502377    -0.752576    -0.612601      37.30
 C       3.958282    -0.434369    -0.918827     104.95
 H       4.259095    -0.532337    -2.033936      22.64
 O       4.255997     0.988312    -0.689366     315.31
 H       5.204501     0.983879    -0.575833      19.24
 C       4.961582    -1.270018    -0.111491      78.25
 H       4.841503    -1.019255     1.021623      23.51
 O       4.685166    -2.762260    -0.226208     289.81
 H       4.790829    -3.001010    -1.176311      29.85
 C       6.476338    -1.120283    -0.500768     100.19
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 O       6.879629     0.280114    -0.471364     284.01
 H       7.242015     0.527273     0.363664      28.52
 H       6.649530    -1.435265    -1.560812      28.85
 H       7.112236    -1.671734     0.235964      29.00
55
name= lig-ACN-Water-frame_68
 C      -4.028934    -0.082055    -3.255278      80.36
 H      -3.978399    -0.995635    -3.732476      25.63
 C      -4.121463     1.298738    -1.279054      74.76
 H      -4.231888     1.311733    -0.224783      25.66
 C      -3.919953     2.440266    -2.034564      11.18
 O      -3.890333     3.750966    -1.499135     191.35
 C      -3.706274     4.052514    -0.129706     119.74
 H      -2.929551     3.463249     0.387858      28.35
 H      -4.591400     3.922987     0.443527      28.50
 H      -3.470621     5.247725    -0.084200      25.20
 C      -3.855311     2.283506    -3.448979       5.40
 O      -3.663587     3.408936    -4.353549      32.78
 H      -4.171300     4.157581    -3.976583      21.69
 C      -3.845899     1.050261    -4.028304      56.12
 H      -3.536633     1.086956    -5.093605      26.01
 C      -4.155756     0.043606    -1.872163      -2.26
 C      -4.087356    -1.245136    -0.971819      67.64
 H      -4.632711    -2.049228    -1.452100      24.79
 O      -4.676780    -0.997662     0.271093     199.85
 H      -4.013664    -0.491675     0.834761      24.62
 C      -2.607570    -1.898497    -0.951718      83.19
 H      -2.431215    -1.842873    -2.081298      26.47
 C      -2.714657    -3.300587    -0.370204     125.93
 O      -3.398222    -4.167456    -1.317878     231.28
 H      -2.674493    -4.694395    -1.694854      29.06
 H      -3.294750    -3.310278     0.561685      26.98
 H      -1.835201    -3.873680    -0.165070      25.89
 C       1.765744    -1.447551    -1.584156      46.14
 H       2.267870    -1.880514    -2.452415      20.76
 C       1.836088    -0.227911     0.559469      80.69
 H       2.435422     0.225099     1.383717      24.76
 C       0.463185    -0.339706     0.714466     -10.78
 O      -0.183426     0.367684     1.719033     229.98
 C       0.522571     0.692775     2.972405     109.62
 H      -0.108140     0.766564     3.832076      26.71
 H       1.255086    -0.041863     3.137946      25.94
 H       0.950758     1.733719     2.750183      25.32
 C      -0.337869    -1.030103    -0.277713     -21.43
 O      -1.763467    -0.944787    -0.221352     136.47
 C       0.311199    -1.580652    -1.411903      57.26
 H      -0.352735    -2.127073    -2.169595      24.24
 C       2.499746    -0.734313    -0.585117      -8.38
 C       3.943025    -0.409091    -0.934964     111.67
 H       4.001289    -0.734710    -2.025049      20.09
 O       4.247411     1.005861    -0.708405     309.85
 H       5.181370     1.075741    -0.464205      17.45
 C       4.962534    -1.321151    -0.097263      90.70
 H       4.792219    -1.035190     1.013708      23.92
 O       4.744562    -2.687569    -0.209023     318.39
 H       4.758307    -2.911549    -1.213327      27.11
 C       6.414916    -1.083264    -0.482424      98.85
 O       6.846456     0.366588    -0.428093     303.10
 H       7.363635     0.336083     0.411213      27.61
 H       6.594571    -1.501862    -1.456996      30.64
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 H       7.026758    -1.727617     0.210615      28.86
55
name= lig-ACN-Water-frame_69
 C      -4.082441    -0.045240    -3.243985      62.50
 H      -4.097313    -1.035409    -3.667758      27.71
 C      -4.110776     1.318674    -1.240447      77.31
 H      -4.036061     1.498298    -0.222089      27.04
 C      -3.934000     2.462151    -2.051974      15.15
 O      -3.926323     3.688327    -1.553186     215.20
 C      -3.797706     4.009707    -0.112044     107.84
 H      -2.951053     3.536019     0.339434      29.78
 H      -4.694832     3.842976     0.451059      27.36
 H      -3.586795     5.208327    -0.233739      24.81
 C      -3.863457     2.429339    -3.512420      13.35
 O      -3.628655     3.427836    -4.323131     151.62
 H      -3.806638     4.414447    -4.025428      20.74
 C      -3.849433     1.082131    -4.067785      44.83
 H      -3.951656     0.929282    -5.133134      22.06
 C      -4.078465     0.024557    -1.813436      18.57
 C      -4.042923    -1.223523    -1.016316      92.57
 H      -4.722669    -1.931368    -1.473363      25.54
 O      -4.683157    -1.030377     0.320666     104.07
 H      -3.981804    -0.666759     1.062756      22.17
 C      -2.640669    -1.838101    -0.997292      87.13
 H      -2.197431    -1.995084    -2.014545      27.65
 C      -2.737665    -3.335477    -0.362784     109.04
 O      -3.402475    -4.209944    -1.335264     220.49
 H      -2.734312    -4.802538    -1.714330      29.05
 H      -3.409177    -3.217574     0.510801      27.24
 H      -1.719998    -3.551694    -0.001985      27.42
 C       1.659015    -1.448831    -1.556555      53.79
 H       2.122147    -1.877597    -2.452224      22.40
 C       1.805747    -0.183267     0.494037       9.90
 H       2.352593     0.427961     1.161119      25.73
 C       0.391090    -0.263918     0.691957       6.84
 O      -0.213360     0.367017     1.776013     192.77
 C       0.566663     0.692324     2.968904     110.10
 H      -0.247866     0.591265     3.687544      26.32
 H       1.333399    -0.005676     3.216015      28.08
 H       1.048004     1.737284     3.033043      25.26
 C      -0.346895    -1.001132    -0.300167     -16.87
 O      -1.757596    -0.958729    -0.211973     150.97
 C       0.307531    -1.606473    -1.394875      86.85
 H      -0.268031    -2.222578    -2.083996      27.22
 C       2.477628    -0.715018    -0.645225       1.51
 C       3.969191    -0.448396    -0.907373     110.73
 H       4.215418    -0.607496    -1.981012      21.12
 O       4.213003     0.999971    -0.699660     279.19
 H       5.227309     1.075986    -0.846973      15.38
 C       4.945285    -1.256470    -0.075865      82.05
 H       4.790484    -1.055968     1.033499      23.98
 O       4.755512    -2.700770    -0.211404     325.22
 H       4.917979    -2.993512    -1.213535      26.47
 C       6.422562    -1.004914    -0.466760     105.55
 O       6.811735     0.370072    -0.365534     308.83
 H       7.137705     0.686368     0.567856      24.14
 H       6.520666    -1.225075    -1.490414      30.14
 H       7.114951    -1.596222     0.167001      28.38
55
name= lig-ACN-Water-frame_70
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 C      -4.063100    -0.030207    -3.228395      37.14
 H      -4.289808    -0.994262    -3.768829      19.34
 C      -4.019849     1.343260    -1.212607      60.90
 H      -4.108767     1.425313    -0.156267      20.14
 C      -3.994344     2.448079    -2.092459       4.17
 O      -3.936910     3.784042    -1.573559     212.16
 C      -3.865447     3.981819    -0.149924     113.67
 H      -3.025067     3.477354     0.268259      28.01
 H      -4.797185     3.635946     0.336530      25.04
 H      -3.775336     5.159910     0.101547      24.58
 C      -3.832894     2.353817    -3.498782      10.77
 O      -3.572427     3.528093    -4.351810     -22.74
 H      -3.954319     4.408835    -3.844187      18.67
 C      -3.968011     1.121883    -4.085211      56.11
 H      -4.102355     1.051927    -5.131574      29.86
 C      -4.049080     0.088156    -1.846457      26.43
 C      -4.061879    -1.199375    -1.019277      69.85
 H      -4.649741    -1.970030    -1.529603      27.26
 O      -4.632672    -1.058082     0.339127     108.88
 H      -3.885130    -0.511374     0.954972      22.13
 C      -2.646011    -1.904538    -0.977364      86.65
 H      -2.294497    -1.919239    -1.999285      29.12
 C      -2.764832    -3.269484    -0.362578     120.99
 O      -3.372735    -4.262078    -1.326098     211.83
 H      -2.552197    -4.707945    -1.749559      27.58
 H      -3.421742    -3.344124     0.541331      26.67
 H      -1.766221    -3.746335    -0.152569      25.27
 C       1.672747    -1.449645    -1.576828      51.44
 H       2.116814    -1.959426    -2.453558      28.16
 C       1.792008    -0.100040     0.420267      81.38
 H       2.323213     0.524749     1.022937      29.28
 C       0.409625    -0.199849     0.649472     -17.09
 O      -0.253739     0.331499     1.767797     180.32
 C       0.555135     0.654702     3.003088      93.96
 H      -0.110496     0.697168     3.913518      25.67
 H       1.379755    -0.063742     3.114104      26.22
 H       0.877955     1.728128     2.821523      24.80
 C      -0.421154    -0.944719    -0.319804      10.29
 O      -1.763338    -0.985672    -0.151950     150.90
 C       0.260323    -1.639625    -1.340357      63.95
 H      -0.211077    -2.206342    -2.086180      25.44
 C       2.425263    -0.688091    -0.711606      14.83
 C       3.933027    -0.439575    -0.925515     108.83
 H       4.170838    -0.725657    -1.949150      23.61
 O       4.181777     0.995908    -0.676140     249.07
 H       5.164897     1.201844    -0.939983      16.24
 C       4.974270    -1.275337    -0.017567      80.33
 H       4.772700    -1.003869     1.044095      24.70
 O       4.742905    -2.724879    -0.200671     319.14
 H       5.020990    -2.968230    -1.177214      26.76
 C       6.446510    -0.940271    -0.461645     102.98
 O       6.789976     0.466599    -0.320323     298.94
 H       7.130765     0.444049     0.718923      21.12
 H       6.548761    -1.213076    -1.469499      29.75
 H       7.107237    -1.649344     0.055054      28.79
55
name= lig-ACN-Water-frame_71
 C      -4.079939    -0.005043    -3.293808      39.91
 H      -4.216632    -1.083749    -3.701427      21.10
 C      -3.957606     1.380724    -1.270648      62.99
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 H      -4.109372     1.437816    -0.162934      21.59
 C      -3.962874     2.587826    -2.048164      12.18
 O      -3.930666     3.882704    -1.627045     222.71
 C      -3.933706     3.925588    -0.157368     110.02
 H      -3.069314     3.436625     0.256497      27.59
 H      -4.834061     3.398513     0.307404      25.39
 H      -3.956759     5.063340     0.048591      25.06
 C      -3.814261     2.431842    -3.498205       7.45
 O      -3.530048     3.463861    -4.291772     124.97
 H      -4.023680     4.398084    -4.214530      20.97
 C      -4.098889     1.116503    -4.107096      58.70
 H      -4.010878     1.057929    -5.166028      25.84
 C      -4.039767     0.097183    -1.856509      38.50
 C      -4.052240    -1.205191    -0.993871     104.46
 H      -4.800633    -1.878006    -1.467188      26.45
 O      -4.563209    -1.053426     0.292571     175.84
 H      -4.011891    -0.406552     0.898443      22.51
 C      -2.668878    -1.871285    -0.946070      93.69
 H      -2.301335    -1.937007    -1.932670      28.67
 C      -2.754107    -3.362450    -0.370692     111.60
 O      -3.326755    -4.274540    -1.301634     249.67
 H      -2.570313    -4.691484    -1.826113      28.04
 H      -3.374184    -3.247250     0.572876      25.63
 H      -1.687342    -3.630251     0.021023      24.97
 C       1.646874    -1.494521    -1.609168      48.33
 H       2.145347    -2.080456    -2.414435      26.84
 C       1.767622     0.028103     0.359998      67.08
 H       2.375452     0.492360     1.070510      26.47
 C       0.375830    -0.173711     0.618294      11.07
 O      -0.275107     0.260205     1.755666     195.66
 C       0.515005     0.650108     2.934674     104.08
 H      -0.199251     0.556705     3.828007      25.08
 H       1.377073    -0.088158     3.097840      25.31
 H       0.989387     1.650924     2.833377      26.31
 C      -0.372794    -0.919633    -0.315710       3.11
 O      -1.844392    -1.037195    -0.072866     131.40
 C       0.254649    -1.634030    -1.366539      72.69
 H      -0.408477    -2.253221    -1.889800      25.27
 C       2.440895    -0.635285    -0.718156     -29.07
 C       3.919762    -0.433036    -0.920101     109.37
 H       4.102519    -0.621806    -1.957163      22.62
 O       4.133304     1.007239    -0.676974     260.91
 H       5.107187     1.133812    -0.593616      15.85
 C       4.951552    -1.322603    -0.057574      89.58
 H       4.840242    -1.125290     1.001861      24.79
 O       4.745753    -2.699126    -0.144119     331.92
 H       4.786153    -3.036098    -1.086584      27.88
 C       6.425451    -0.937451    -0.473358     100.60
 O       6.787537     0.541832    -0.247547     254.90
 H       7.472313     0.637432     0.546580      22.40
 H       6.535667    -1.099159    -1.523925      28.69
 H       7.159135    -1.438597     0.115357      28.51
55
name= lig-ACN-Water-frame_72
 C      -4.150420    -0.015784    -3.282253      45.81
 H      -4.080084    -1.001746    -3.866700      28.86
 C      -3.971573     1.443352    -1.334470      50.66
 H      -3.859400     1.539001    -0.189387      20.26
 C      -3.867521     2.588272    -2.115819      16.97
 O      -3.909608     3.936555    -1.601231     194.04
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 C      -3.984755     3.939345    -0.152117     112.25
 H      -3.016551     3.590489     0.277525      28.63
 H      -4.899649     3.312896     0.190256      27.78
 H      -4.138701     4.952456     0.204671      27.22
 C      -3.930492     2.416512    -3.468567      16.90
 O      -3.472630     3.437722    -4.326298     124.39
 H      -3.696193     4.313646    -3.921074      20.06
 C      -4.089816     1.202765    -4.071438      56.88
 H      -4.176617     1.140400    -5.151810      22.17
 C      -4.021378     0.109799    -1.903651      11.93
 C      -4.032136    -1.162234    -1.056068      60.86
 H      -4.646443    -1.950230    -1.581141      23.00
 O      -4.581066    -1.019803     0.317927     202.83
 H      -3.896172    -0.631209     0.879642      24.86
 C      -2.642762    -1.905122    -0.942301      78.14
 H      -2.186219    -1.911394    -1.880068      27.37
 C      -2.710870    -3.352743    -0.326500     106.40
 O      -3.305586    -4.298922    -1.292275     238.97
 H      -2.587806    -4.734308    -1.767652      28.73
 H      -3.457966    -3.461678     0.514067      24.81
 H      -1.627021    -3.701778    -0.028668      23.61
 C       1.642387    -1.480117    -1.547519      43.38
 H       2.128794    -2.081121    -2.337296      22.33
 C       1.728444     0.072027     0.321403      53.31
 H       2.284810     0.732306     1.020770      23.20
 C       0.370573    -0.155100     0.585725      -4.29
 O      -0.308830     0.211771     1.741727     201.80
 C       0.493840     0.621520     2.856485     109.36
 H      -0.301495     0.644378     3.699804      23.93
 H       1.312486    -0.166743     3.137549      24.36
 H       0.821435     1.652309     2.791187      25.04
 C      -0.476034    -0.976900    -0.324720       5.17
 O      -1.773446    -1.080062    -0.023601     140.45
 C       0.235314    -1.598604    -1.387000      75.76
 H      -0.129101    -2.356708    -2.082969      24.55
 C       2.366895    -0.650962    -0.752743      25.67
 C       3.924931    -0.407491    -0.939917     110.77
 H       4.216627    -0.597401    -1.932947      23.65
 O       4.124210     0.999777    -0.650672     303.06
 H       5.018191     1.123478    -0.370479      18.68
 C       4.930113    -1.227422    -0.089989      86.88
 H       4.752375    -0.904392     0.914971      25.48
 O       4.734638    -2.729608    -0.104767     329.02
 H       4.842431    -2.995458    -1.036411      28.71
 C       6.434011    -0.857947    -0.457976     102.76
 O       6.763148     0.551326    -0.230996     322.81
 H       7.100942     0.563626     0.722814      26.63
 H       6.650985    -1.054617    -1.521924      29.56
 H       7.013935    -1.583703     0.057517      30.31
55
name= lig-ACN-Water-frame_73
 C      -4.186114     0.037674    -3.306415      65.44
 H      -4.356344    -0.948959    -3.775207      25.43
 C      -3.945503     1.403690    -1.317081      55.28
 H      -3.805469     1.423790    -0.172108      21.28
 C      -3.874898     2.611562    -2.085556       7.90
 O      -3.844054     3.889105    -1.570470     193.08
 C      -4.006413     3.997402    -0.111649     111.90
 H      -3.069566     3.629029     0.438767      27.98
 H      -4.789338     3.228270     0.277673      27.53
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 H      -4.292091     4.973376     0.072761      28.00
 C      -3.920645     2.489444    -3.553308       7.97
 O      -3.451803     3.471049    -4.360305      27.94
 H      -3.768035     4.322858    -4.085758      20.80
 C      -4.098592     1.157279    -4.090507      54.37
 H      -4.200081     1.157583    -5.200332      23.05
 C      -4.030034     0.152788    -1.905771      29.55
 C      -3.974890    -1.169243    -1.023292      65.87
 H      -4.699971    -1.860416    -1.559362      22.83
 O      -4.619602    -1.002613     0.284859     173.91
 H      -4.067377    -0.531853     0.843837      28.00
 C      -2.581377    -1.920015    -0.911863     100.74
 H      -2.201267    -2.018368    -1.898928      27.01
 C      -2.722610    -3.337278    -0.343318     115.66
 O      -3.302813    -4.314437    -1.278228     215.29
 H      -2.521360    -4.683421    -1.755844      27.19
 H      -3.272540    -3.182656     0.627890      25.98
 H      -1.655444    -3.737192    -0.053291      23.66
 C       1.623087    -1.475506    -1.531852      60.57
 H       2.123143    -2.007871    -2.349457      20.74
 C       1.667230     0.056839     0.289242      44.15
 H       2.200207     0.929272     0.842782      21.37
 C       0.297814    -0.214540     0.521429      24.74
 O      -0.356558     0.183198     1.687186     202.88
 C       0.433234     0.632454     2.866737      93.90
 H      -0.187057     0.726041     3.811671      24.79
 H       1.346216    -0.110102     3.022237      25.50
 H       0.929622     1.528918     2.574717      26.16
 C      -0.391670    -1.003359    -0.349985      13.70
 O      -1.773177    -1.150828    -0.006299     162.60
 C       0.219018    -1.630946    -1.424273      71.22
 H      -0.470395    -2.212933    -2.116526      23.19
 C       2.425465    -0.589948    -0.701759      11.14
 C       3.871143    -0.394032    -1.006773     121.06
 H       3.996519    -0.581513    -2.019039      21.12
 O       4.124670     1.011917    -0.601817     273.41
 H       5.127295     1.096002    -0.594636      16.63
 C       4.909701    -1.191585    -0.068760      92.46
 H       4.754699    -0.934485     0.943795      25.14
 O       4.738100    -2.646432    -0.084425     322.66
 H       4.943836    -2.964045    -0.984716      30.31
 C       6.387250    -0.858249    -0.456962     102.73
 O       6.739071     0.542021    -0.195240     309.07
 H       7.134895     0.562386     0.676785      28.71
 H       6.522351    -1.018312    -1.572201      29.48
 H       7.073454    -1.393184     0.149274      29.56
55
name= lig-ACN-Water-frame_74
 C      -4.220882     0.028145    -3.289198      25.23
 H      -4.537000    -0.894972    -3.698392      21.62
 C      -3.877660     1.415760    -1.284574      51.30
 H      -3.845483     1.562731    -0.183356      21.13
 C      -3.939627     2.557301    -2.091803      11.65
 O      -3.755559     3.827790    -1.518383     218.64
 C      -4.006209     4.020217    -0.081950     115.39
 H      -3.017697     3.962510     0.525785      25.75
 H      -4.867332     3.386767     0.296526      24.97
 H      -4.271946     4.993922     0.019910      27.03
 C      -3.816706     2.474924    -3.531029      22.75
 O      -3.476918     3.568952    -4.399868     139.14
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 H      -4.007947     4.391615    -4.235414      24.37
 C      -4.118970     1.244124    -4.172122      47.02
 H      -4.124843     1.009223    -5.271845      25.43
 C      -4.024641     0.085635    -1.863903      32.46
 C      -3.982850    -1.164463    -1.017908      92.50
 H      -4.571680    -1.987266    -1.546428      27.85
 O      -4.659405    -1.002439     0.235929     167.50
 H      -4.153766    -0.428676     0.877012      25.75
 C      -2.624238    -1.893725    -0.947884      96.71
 H      -2.193345    -1.847991    -1.957529      30.10
 C      -2.716988    -3.342038    -0.357422     111.29
 O      -3.338188    -4.293624    -1.222609     200.36
 H      -2.634851    -4.719867    -1.838467      26.87
 H      -3.477501    -3.345265     0.457610      26.70
 H      -1.655132    -3.622418     0.009676      25.65
 C       1.659013    -1.481400    -1.598438      73.11
 H       2.192133    -1.948631    -2.411342      26.85
 C       1.650726     0.096301     0.305034      60.00
 H       2.156498     0.860785     1.037291      22.98
 C       0.330116    -0.226171     0.592098     -10.33
 O      -0.430377     0.183764     1.676772     182.42
 C       0.441826     0.652773     2.785202     105.14
 H      -0.359696     0.725895     3.541321      25.51
 H       1.164190    -0.210079     3.111904      25.49
 H       0.847003     1.648698     2.732189      26.45
 C      -0.441358    -1.073153    -0.366335      10.15
 O      -1.743023    -1.213612    -0.023700     164.26
 C       0.265288    -1.657724    -1.454803      74.32
 H      -0.198327    -2.297705    -2.314920      24.92
 C       2.319593    -0.642350    -0.727521      21.00
 C       3.859853    -0.334610    -0.948465     110.30
 H       4.136715    -0.469175    -1.935302      25.83
 O       4.124248     1.053167    -0.618320     258.79
 H       5.141112     1.240982    -0.667037      17.44
 C       4.866476    -1.189077    -0.071955     101.55
 H       4.649300    -0.812197     0.894566      27.08
 O       4.735484    -2.561103    -0.070190     344.42
 H       4.855728    -2.919929    -1.000388      28.09
 C       6.336855    -0.865823    -0.433858      90.55
 O       6.727755     0.552610    -0.195627     276.94
 H       7.309050     0.583459     0.623722      24.86
 H       6.511097    -1.086485    -1.556641      29.48
 H       6.946792    -1.635228     0.035616      30.23
55
name= lig-ACN-Water-frame_75
 C      -4.242298     0.101345    -3.286899      84.36
 H      -4.361174    -0.767800    -3.836692      22.49
 C      -3.865536     1.352057    -1.298001      65.14
 H      -3.732158     1.463055    -0.257779      24.84
 C      -3.858928     2.545384    -2.103047       5.45
 O      -3.695600     3.785648    -1.487080     202.96
 C      -3.986979     4.081145    -0.094208     115.86
 H      -3.069929     3.734262     0.543327      26.31
 H      -4.746116     3.422329     0.339647      25.99
 H      -4.290795     5.075297    -0.047573      27.90
 C      -3.787280     2.497062    -3.561335       8.39
 O      -3.548539     3.617432    -4.366150      37.47
 H      -3.789904     4.509869    -3.881178      22.28
 C      -4.087114     1.208567    -4.072863      37.39
 H      -4.234631     1.311027    -5.179167      24.29
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 C      -4.019749     0.133349    -1.903658      36.53
 C      -4.050879    -1.197827    -1.067288      78.67
 H      -4.719595    -1.897166    -1.649506      25.14
 O      -4.727702    -1.019666     0.227934     143.13
 H      -3.986327    -0.668707     0.961586      22.99
 C      -2.654804    -1.903023    -0.971793      89.35
 H      -2.248197    -1.955890    -2.031046      27.74
 C      -2.775059    -3.314439    -0.356470     115.13
 O      -3.394567    -4.315580    -1.220446     207.71
 H      -2.628685    -4.636317    -1.817647      27.29
 H      -3.284922    -3.170397     0.618492      26.30
 H      -1.751143    -3.713181    -0.092407      25.41
 C       1.682876    -1.464536    -1.651403      56.83
 H       2.200681    -2.010665    -2.419293      27.90
 C       1.648095     0.039358     0.331115      26.99
 H       2.347100     0.646655     0.981088      25.09
 C       0.282890    -0.295628     0.565332      20.27
 O      -0.416209     0.216821     1.652257     205.81
 C       0.315061     0.663090     2.792189     117.00
 H      -0.281891     0.822491     3.664874      28.05
 H       1.175899    -0.067020     3.036343      27.11
 H       0.858673     1.547202     2.435169      29.61
 C      -0.358874    -1.112386    -0.362402       6.01
 O      -1.748064    -1.226939    -0.037921     136.23
 C       0.285806    -1.696818    -1.478288      72.18
 H      -0.304636    -2.433593    -2.139326      26.16
 C       2.365183    -0.566068    -0.735678     -64.46
 C       3.836127    -0.293822    -0.911083     125.17
 H       4.023082    -0.531571    -1.904542      22.35
 O       4.100145     1.150567    -0.647893     248.48
 H       5.089215     1.184984    -0.484942      16.51
 C       4.831441    -1.063389    -0.023100      86.71
 H       4.749089    -0.863329     1.023202      26.02
 O       4.666887    -2.586857    -0.049687     299.70
 H       4.967005    -2.947712    -0.984668      26.38
 C       6.312675    -0.843322    -0.446298      93.23
 O       6.754978     0.517509    -0.228518     287.44
 H       7.142788     0.485431     0.787295      21.50
 H       6.421775    -1.009741    -1.577338      25.78
 H       6.947452    -1.481741     0.207426      27.92
55
name= lig-ACN-Water-frame_76
 C      -4.204642     0.075882    -3.340704      43.84
 H      -4.378652    -0.882573    -3.787148      31.74
 C      -3.847803     1.388270    -1.317210      65.20
 H      -3.739975     1.373663    -0.295898      26.08
 C      -3.685028     2.556874    -2.037491      15.31
 O      -3.647483     3.822773    -1.519798     230.00
 C      -3.941412     4.039217    -0.107494     116.38
 H      -3.017243     3.917103     0.549691      28.07
 H      -4.808007     3.532411     0.190918      28.75
 H      -4.073994     5.139088    -0.046095      26.68
 C      -3.817021     2.559159    -3.453751      27.99
 O      -3.631261     3.586140    -4.296439     123.53
 H      -3.813702     4.569985    -3.912908      16.49
 C      -4.039294     1.317316    -4.088874      57.64
 H      -4.301657     1.091052    -5.134340      24.67
 C      -4.056379     0.083992    -1.916202      15.78
 C      -4.111408    -1.176029    -1.111707      74.75
 H      -4.767550    -1.923867    -1.624115      24.45
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 O      -4.773620    -1.068060     0.209191     147.01
 H      -4.102419    -0.748756     0.963976      23.41
 C      -2.699964    -1.952608    -0.985652      79.68
 H      -2.221847    -2.032938    -2.035683      26.37
 C      -2.807123    -3.331821    -0.352613     116.92
 O      -3.464881    -4.322772    -1.223406     202.29
 H      -2.781184    -4.715598    -1.791810      29.74
 H      -3.403650    -3.323687     0.571945      26.04
 H      -1.765284    -3.631794    -0.171108      26.15
 C       1.684417    -1.404895    -1.624701      46.17
 H       2.275387    -1.954995    -2.344096      23.12
 C       1.681403    -0.083205     0.362231      53.97
 H       2.046419     0.632806     1.057970      25.63
 C       0.343507    -0.293072     0.565261      -0.37
 O      -0.464608     0.202347     1.592241     203.64
 C       0.305501     0.715483     2.793135     106.45
 H      -0.495200     0.871707     3.477938      26.02
 H       0.992576    -0.074077     3.154667      26.43
 H       0.771450     1.738398     2.696678      24.53
 C      -0.396374    -1.145586    -0.369019      -0.23
 O      -1.767833    -1.207572    -0.102405     132.66
 C       0.317715    -1.733553    -1.436058      74.88
 H      -0.201238    -2.448620    -2.095002      23.39
 C       2.361149    -0.543834    -0.781828      43.95
 C       3.846802    -0.227543    -0.921235      91.91
 H       4.174642    -0.420319    -1.899912      24.41
 O       4.083802     1.206867    -0.658288     269.79
 H       5.023410     1.366706    -0.663658      21.84
 C       4.839005    -1.141875     0.032186      76.91
 H       4.629254    -0.726459     1.025421      26.39
 O       4.568544    -2.521772     0.004277     353.59
 H       4.885731    -2.914741    -0.923131      25.58
 C       6.290596    -0.832028    -0.438593      96.77
 O       6.781829     0.527297    -0.249738     270.88
 H       7.334368     0.596878     0.709326      21.93
 H       6.402895    -1.130774    -1.538691      29.24
 H       6.967908    -1.616928     0.049459      29.47
55
name= lig-ACN-Water-frame_77
 C      -4.114543     0.096731    -3.362693      49.30
 H      -4.405590    -0.767635    -4.015647      18.01
 C      -3.797923     1.335707    -1.255444      54.43
 H      -3.866070     1.437756    -0.213151      21.05
 C      -3.608363     2.580414    -2.008027      -0.12
 O      -3.571599     3.915832    -1.522288     228.91
 C      -3.864394     4.048232    -0.141720     118.43
 H      -3.072666     3.574367     0.476367      27.46
 H      -4.700540     3.507644     0.155439      28.53
 H      -4.104252     5.168130     0.061121      24.86
 C      -3.821303     2.484585    -3.411469      14.74
 O      -3.701181     3.624674    -4.258929      93.12
 H      -4.274956     4.419901    -3.918776      15.08
 C      -4.055475     1.281178    -4.091864      45.05
 H      -4.041329     1.579463    -5.126761      25.11
 C      -4.076646     0.134402    -1.950097      23.56
 C      -4.114938    -1.232234    -1.087550      80.04
 H      -4.692986    -1.949237    -1.698095      24.66
 O      -4.802107    -1.119671     0.177255     180.40
 H      -4.276865    -0.562916     0.714027      27.91
 C      -2.745437    -1.948760    -1.004076      86.93
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 H      -2.385080    -2.051229    -2.109717      25.97
 C      -2.835568    -3.412187    -0.359293     121.67
 O      -3.528627    -4.319556    -1.232030     203.70
 H      -2.881136    -4.689732    -1.863517      28.73
 H      -3.441462    -3.307038     0.558429      26.58
 H      -1.881208    -3.781610    -0.045495      26.56
 C       1.687589    -1.415403    -1.611240      81.94
 H       2.126619    -1.862533    -2.509417      16.64
 C       1.714717    -0.080103     0.441652      46.45
 H       2.291735     0.506753     1.046387      21.26
 C       0.275190    -0.360203     0.542487      11.81
 O      -0.438436     0.227471     1.575641     220.98
 C       0.202401     0.747134     2.786187     107.86
 H      -0.601320     0.866461     3.501782      25.25
 H       0.882591     0.048520     3.214907      26.78
 H       0.773545     1.709145     2.578534      24.84
 C      -0.450930    -1.145305    -0.381122      21.62
 O      -1.820071    -1.171995    -0.189215     166.93
 C       0.324858    -1.765681    -1.385616      53.72
 H      -0.045632    -2.407678    -2.125754      19.10
 C       2.404257    -0.527629    -0.742758      43.74
 C       3.921221    -0.219918    -0.948642      90.94
 H       4.166728    -0.403090    -1.979135      22.44
 O       4.067571     1.211809    -0.631221     262.66
 H       4.995181     1.439961    -0.915861      19.64
 C       4.805223    -1.060999     0.015530      79.44
 H       4.702068    -0.780500     1.101287      23.35
 O       4.462202    -2.479554     0.067817     321.49
 H       4.582175    -2.842964    -0.897020      27.86
 C       6.317804    -0.893793    -0.422333      87.69
 O       6.802643     0.539963    -0.281483     263.99
 H       7.097331     0.546648     0.780089      23.93
 H       6.307701    -0.975489    -1.535452      30.18
 H       7.057155    -1.601849     0.117372      28.82
55
name= lig-ACN-Water-frame_78
 C      -4.086302     0.093893    -3.367964      25.90
 H      -4.173637    -0.973819    -3.803968      30.39
 C      -3.765009     1.387445    -1.238660      54.09
 H      -3.736505     1.275780    -0.142446      21.91
 C      -3.671017     2.578179    -1.988812      15.00
 O      -3.493602     3.917258    -1.552017     217.89
 C      -3.807059     4.027108    -0.109584     115.00
 H      -2.996606     3.663609     0.473007      27.72
 H      -4.732989     3.580031     0.044861      26.83
 H      -3.859088     5.185866     0.163692      25.23
 C      -3.769127     2.553066    -3.437668      20.73
 O      -3.796161     3.631656    -4.206406     127.99
 H      -4.159593     4.454211    -3.860829      19.84
 C      -4.006462     1.309596    -4.096242      64.04
 H      -4.189222     1.112181    -5.126629      23.87
 C      -4.012548     0.112130    -1.918633     -16.52
 C      -4.132111    -1.249903    -1.155894      78.38
 H      -4.807125    -1.915681    -1.685920      25.39
 O      -4.821956    -1.148926     0.142742     129.53
 H      -4.352486    -0.643855     0.784366      29.25
 C      -2.728622    -2.004723    -1.025703      90.69
 H      -2.305549    -2.112663    -2.100177      28.54
 C      -2.881507    -3.390797    -0.357058     121.47
 O      -3.574650    -4.336961    -1.270050     129.16
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 H      -2.834268    -4.607160    -1.927061      28.22
 H      -3.476409    -3.284664     0.568186      27.32
 H      -1.920173    -3.786962    -0.186564      26.54
 C       1.692905    -1.411252    -1.553376      45.70
 H       2.207351    -1.811472    -2.434600      26.33
 C       1.685074    -0.096381     0.418483      69.06
 H       2.045468     0.387662     1.244255      22.69
 C       0.331448    -0.340117     0.597240       9.30
 O      -0.475640     0.250053     1.576853     232.86
 C       0.128277     0.758136     2.776137     115.79
 H      -0.691138     1.041664     3.475832      25.09
 H       0.816322     0.098887     3.169887      27.68
 H       0.647806     1.737482     2.528411      25.40
 C      -0.424752    -1.131756    -0.389318      -3.37
 O      -1.887475    -1.121083    -0.254462     133.41
 C       0.307930    -1.777337    -1.409470      55.00
 H      -0.234818    -2.390139    -2.027857      21.61
 C       2.419717    -0.591756    -0.676304      47.40
 C       3.858024    -0.224826    -0.924990      99.31
 H       4.134481    -0.466607    -1.971888      21.53
 O       4.082322     1.217081    -0.613445     241.44
 H       5.082047     1.414054    -0.774755      18.87
 C       4.852209    -0.995261     0.000038      78.84
 H       4.675866    -0.441778     1.001193      22.35
 O       4.361473    -2.436553     0.094309     317.24
 H       4.560496    -2.796222    -0.811033      28.28
 C       6.321960    -0.858634    -0.449050     102.12
 O       6.791659     0.481704    -0.291905     320.02
 H       6.999249     0.643313     0.681648      29.43
 H       6.535383    -1.262002    -1.451327      30.35
 H       6.915014    -1.587968     0.246368      28.23
55
name= lig-ACN-Water-frame_79
 C      -4.032330     0.111566    -3.246470      39.23
 H      -4.138232    -0.832228    -3.896290      23.35
 C      -3.773002     1.368540    -1.282165      59.59
 H      -3.500716     1.581956    -0.190982      26.49
 C      -3.721668     2.584491    -2.050259      13.49
 O      -3.453394     3.843909    -1.508310     220.62
 C      -3.734029     4.040204    -0.113586     120.28
 H      -3.029299     3.606229     0.495979      28.37
 H      -4.674372     3.613804     0.214151      27.29
 H      -3.834534     5.213971    -0.060285      25.25
 C      -3.808027     2.509880    -3.447198      10.66
 O      -3.861536     3.695735    -4.241561      94.85
 H      -4.092286     4.466312    -3.726364      23.26
 C      -3.939611     1.250571    -4.076340      55.96
 H      -4.199229     1.376097    -5.104809      29.36
 C      -3.914883     0.120103    -1.886402      40.32
 C      -4.112383    -1.221733    -1.196397      62.79
 H      -4.722582    -1.825439    -1.838568      22.50
 O      -4.830048    -1.171845     0.099780     141.73
 H      -4.077190    -0.774125     0.734287      24.42
 C      -2.749111    -2.004936    -1.081073      79.39
 H      -2.281292    -2.235430    -2.091409      27.16
 C      -2.898680    -3.379718    -0.385320     114.80
 O      -3.577391    -4.332060    -1.312722     163.55
 H      -2.877294    -4.700923    -1.930455      28.69
 H      -3.531581    -3.394019     0.530466      26.84
 H      -1.939564    -3.720189    -0.082452      27.70
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 C       1.676749    -1.472697    -1.548480      52.77
 H       2.284276    -2.013924    -2.272044      27.88
 C       1.658065    -0.095039     0.501365      53.21
 H       2.269134     0.587542     1.081689      20.61
 C       0.235991    -0.327964     0.588673      16.33
 O      -0.551773     0.233422     1.555916     203.62
 C       0.115028     0.823740     2.775376     107.64
 H      -0.806816     0.931813     3.416789      25.54
 H       0.649411     0.099027     3.275958      28.75
 H       0.681242     1.770518     2.640147      25.83
 C      -0.457519    -1.106117    -0.362201      26.72
 O      -1.824798    -1.072498    -0.278217     137.10
 C       0.288524    -1.711996    -1.408114      83.67
 H      -0.047434    -2.346917    -2.182446      22.37
 C       2.347838    -0.637132    -0.617069      12.74
 C       3.834516    -0.205275    -0.881636      91.76
 H       4.000193    -0.344392    -2.003044      18.52
 O       4.076939     1.221281    -0.624325     267.23
 H       5.052992     1.265131    -0.579899      20.45
 C       4.798475    -1.032383    -0.034538      90.85
 H       4.837372    -0.675910     1.068913      22.46
 O       4.346393    -2.325578     0.110804     362.36
 H       4.584053    -2.810160    -0.685554      30.26
 C       6.320504    -0.930215    -0.411189      98.77
 O       6.777579     0.471051    -0.319746     303.54
 H       7.158011     0.482955     0.520270      31.85
 H       6.514034    -1.197313    -1.443229      29.80
 H       6.932012    -1.557021     0.327609      28.30
55
name= lig-ACN-Water-frame_80
 C      -3.956546     0.093056    -3.301030      41.26
 H      -4.275593    -0.885073    -3.710101      28.36
 C      -3.726645     1.428303    -1.269124      65.69
 H      -3.660770     1.416081    -0.117059      23.23
 C      -3.711650     2.546303    -2.062160      16.23
 O      -3.448784     3.759305    -1.491131     226.37
 C      -3.678319     4.073906    -0.100431     114.67
 H      -2.900467     3.751419     0.482551      28.86
 H      -4.674593     3.664138     0.214113      26.44
 H      -3.707133     5.206229     0.018975      26.00
 C      -3.897637     2.575777    -3.506123      16.33
 O      -3.885755     3.650592    -4.286693     -22.39
 H      -4.364381     4.497397    -3.903323      17.07
 C      -3.915781     1.281061    -4.063362      62.95
 H      -3.941897     1.091691    -5.133243      24.79
 C      -3.882125     0.150455    -1.859085       2.47
 C      -4.041003    -1.212455    -1.163667      88.97
 H      -4.732663    -1.782260    -1.799636      26.68
 O      -4.769213    -1.179183     0.035645     145.38
 H      -4.302481    -0.649062     0.890675      20.41
 C      -2.716072    -1.956879    -1.076402     100.43
 H      -2.372585    -1.999980    -2.132777      28.64
 C      -2.908240    -3.405471    -0.414876     116.70
 O      -3.541401    -4.315378    -1.353311     201.61
 H      -2.803526    -4.650957    -1.869685      31.22
 H      -3.602108    -3.189437     0.435173      25.60
 H      -1.958075    -3.824983    -0.102371      27.03
 C       1.691868    -1.521160    -1.480936      55.75
 H       2.159762    -2.110416    -2.256230      17.30
 C       1.595733    -0.093128     0.511373      61.87
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 H       1.982714     0.731202     1.204445      20.15
 C       0.217438    -0.291222     0.603641      10.20
 O      -0.599517     0.263997     1.593264     219.69
 C       0.020442     0.813906     2.774793     110.01
 H      -0.739034     1.233854     3.474449      25.14
 H       0.736196     0.139658     3.174016      27.73
 H       0.603424     1.663252     2.428496      25.67
 C      -0.442791    -1.096273    -0.413894      14.50
 O      -1.854656    -1.089748    -0.305568     163.53
 C       0.287093    -1.673938    -1.448019      68.56
 H      -0.377907    -2.273451    -2.103522      23.60
 C       2.334940    -0.606791    -0.584136      34.12
 C       3.781033    -0.188402    -0.866871      85.90
 H       4.014543    -0.480737    -1.968878      22.09
 O       4.036340     1.224397    -0.625791     265.56
 H       4.976827     1.312499    -0.517708      21.91
 C       4.812959    -0.997712     0.020472      83.80
 H       4.621569    -0.443802     1.013663      23.55
 O       4.348105    -2.385496     0.121973     366.80
 H       4.555301    -2.778682    -0.789356      28.53
 C       6.294560    -0.981506    -0.414217     102.93
 O       6.776808     0.456423    -0.317806     312.27
 H       6.992293     0.610222     0.596417      31.91
 H       6.407206    -1.307570    -1.430784      31.34
 H       6.908791    -1.661599     0.221530      30.28
55
name= lig-ACN-Water-frame_81
 C      -3.909209     0.111928    -3.309990      66.01
 H      -3.922948    -0.803714    -3.829060      24.82
 C      -3.702289     1.362531    -1.244985      57.73
 H      -3.711022     1.547716    -0.138977      21.11
 C      -3.702352     2.569158    -2.031822      12.11
 O      -3.441552     3.826156    -1.508679     204.74
 C      -3.628930     4.083500    -0.087389     121.30
 H      -2.853817     3.726701     0.526429      27.55
 H      -4.615256     3.670758     0.350148      27.12
 H      -3.699696     5.151909    -0.142033      27.63
 C      -3.930860     2.517899    -3.466587      19.08
 O      -3.918673     3.650702    -4.383270      -7.71
 H      -4.297579     4.563306    -3.934182      15.63
 C      -3.924033     1.253899    -4.120426      50.49
 H      -3.996416     1.251424    -5.233139      26.14
 C      -3.891957     0.143587    -1.918570      44.28
 C      -4.014328    -1.171475    -1.185650      76.19
 H      -4.568524    -1.885541    -1.840212      24.38
 O      -4.767913    -1.158942     0.071230     163.02
 H      -4.105450    -0.589279     0.740340      20.91
 C      -2.649536    -1.971006    -1.098117      95.08
 H      -2.235978    -2.140249    -2.087884      26.57
 C      -2.892165    -3.344659    -0.455935     113.04
 O      -3.508392    -4.303338    -1.395090     194.38
 H      -2.792551    -4.578125    -2.030391      28.58
 H      -3.600698    -3.376364     0.411192      25.30
 H      -1.927077    -3.742136    -0.039571      24.97
 C       1.687502    -1.510760    -1.434502      35.00
 H       2.370333    -1.883644    -2.179499      17.11
 C       1.547308    -0.016432     0.467823      52.26
 H       2.113078     0.592665     1.311296      21.60
 C       0.157218    -0.291455     0.612821      16.06
 O      -0.670676     0.254436     1.598645     214.87
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 C       0.021521     0.859149     2.732669     117.88
 H      -0.838624     1.101200     3.359751      25.55
 H       0.519726     0.099533     3.355966      26.50
 H       0.579039     1.740955     2.514809      27.49
 C      -0.497439    -1.027341    -0.408601      24.57
 O      -1.841951    -1.113594    -0.286218     177.91
 C       0.253962    -1.677741    -1.434777      97.34
 H      -0.071703    -2.361686    -2.307942      21.90
 C       2.320356    -0.591216    -0.588533      26.15
 C       3.792500    -0.237190    -0.841024      86.49
 H       4.033636    -0.393663    -1.987738      20.10
 O       3.968548     1.246770    -0.632355     249.77
 H       4.969089     1.323841    -0.727872      19.58
 C       4.757679    -1.015509     0.089677      87.79
 H       4.783372    -0.700789     1.166176      24.23
 O       4.378134    -2.467223     0.144574     338.62
 H       4.656740    -2.844639    -0.792023      28.07
 C       6.243111    -0.905517    -0.405104     113.61
 O       6.767797     0.398965    -0.300015     290.97
 H       7.012504     0.558080     0.695942      26.48
 H       6.371170    -1.164220    -1.444386      31.57
 H       6.827290    -1.606510     0.187374      30.78
55
name= lig-ACN-Water-frame_82
 C      -3.874326     0.079735    -3.388265      55.81
 H      -3.713627    -0.838594    -3.836878      30.34
 C      -3.739890     1.386370    -1.291556      59.03
 H      -3.578416     1.323413    -0.245655      22.10
 C      -3.701794     2.587123    -2.058444      17.51
 O      -3.461664     3.914776    -1.531384     194.74
 C      -3.590332     4.118401    -0.102316     118.35
 H      -2.740025     3.664077     0.400397      27.26
 H      -4.570408     3.583253     0.238633      25.81
 H      -3.687645     5.113016     0.113043      27.63
 C      -3.885096     2.534945    -3.486005      26.95
 O      -3.959539     3.592163    -4.393011     -22.36
 H      -4.263117     4.469636    -3.888117      18.69
 C      -3.952898     1.297295    -4.129403      58.19
 H      -4.146771     1.336991    -5.243434      26.72
 C      -3.885134     0.137356    -1.941819      -0.70
 C      -4.023595    -1.245363    -1.245025      69.10
 H      -4.830363    -1.787500    -1.809901      21.73
 O      -4.752446    -1.112350     0.050409     111.98
 H      -4.125708    -0.724259     0.839013      18.73
 C      -2.677293    -1.967658    -1.119547     102.53
 H      -2.190727    -2.054827    -2.060387      28.47
 C      -2.858215    -3.364743    -0.458093     113.86
 O      -3.478492    -4.271713    -1.427379     193.80
 H      -2.689369    -4.550704    -2.039410      27.50
 H      -3.558985    -3.159443     0.384402      25.51
 H      -1.822084    -3.736866    -0.132218      23.95
 C       1.665736    -1.424465    -1.468088      44.82
 H       2.094802    -2.003661    -2.273518      23.08
 C       1.523257     0.045113     0.463253      60.36
 H       2.136833     0.676145     1.239141      20.75
 C       0.155034    -0.248038     0.559876      16.88
 O      -0.682942     0.229756     1.570017     217.73
 C      -0.055146     0.892378     2.765354     108.21
 H      -0.833286     1.294620     3.363492      25.80
 H       0.650111     0.120022     3.230599      25.11
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 H       0.599769     1.672695     2.456388      26.72
 C      -0.470313    -1.046155    -0.453086      20.30
 O      -1.852996    -1.134617    -0.221677     177.72
 C       0.313583    -1.685013    -1.382537      52.05
 H      -0.280053    -2.350071    -2.126163      18.05
 C       2.282023    -0.549952    -0.564358      41.22
 C       3.749872    -0.237147    -0.750358      97.94
 H       4.048858    -0.602421    -1.848045      20.37
 O       3.943470     1.229876    -0.629882     250.01
 H       4.900339     1.512923    -0.903244      20.03
 C       4.733503    -1.132381     0.124886      97.39
 H       4.523143    -0.719674     1.117660      25.38
 O       4.440530    -2.493895     0.168864     333.73
 H       4.688538    -2.867424    -0.787779      26.48
 C       6.186510    -0.915299    -0.381017     102.07
 O       6.769333     0.434037    -0.264532     316.22
 H       7.251407     0.528028     0.724568      24.59
 H       6.117496    -1.099365    -1.459664      31.57
 H       6.821972    -1.646482     0.058671      29.54
55
name= lig-ACN-Water-frame_83
 C      -3.854192     0.091886    -3.427892      70.39
 H      -4.019241    -0.843342    -3.937200      24.99
 C      -3.775704     1.423696    -1.373816      56.98
 H      -3.688616     1.496095    -0.339141      22.44
 C      -3.689446     2.667946    -2.088764      26.71
 O      -3.513854     3.949490    -1.593639     185.48
 C      -3.572954     4.084935    -0.123890     119.09
 H      -2.652642     3.718257     0.417672      26.74
 H      -4.501640     3.552199     0.323249      27.01
 H      -3.637110     5.096550    -0.003863      27.48
 C      -3.841278     2.543595    -3.499332      39.06
 O      -3.999304     3.592021    -4.368807     115.27
 H      -4.490512     4.368319    -4.005782      21.92
 C      -3.962318     1.270830    -4.116028      60.88
 H      -4.079791     1.190119    -5.233758      23.98
 C      -3.856985     0.119568    -2.030914       8.86
 C      -4.083439    -1.202552    -1.224458      86.19
 H      -4.658661    -1.919514    -1.853432      25.98
 O      -4.746072    -1.104068    -0.024604     214.42
 H      -4.214946    -0.553007     0.624913      23.51
 C      -2.689937    -1.969020    -1.110875      89.72
 H      -2.326791    -1.997862    -2.106016      28.30
 C      -2.822440    -3.368302    -0.486294     120.39
 O      -3.462122    -4.249112    -1.427851     212.10
 H      -2.703454    -4.634702    -1.968612      27.91
 H      -3.453891    -3.405249     0.430705      25.91
 H      -1.821562    -3.856810    -0.110071      24.70
 C       1.665648    -1.379053    -1.540089      27.04
 H       2.401667    -1.752355    -2.262101      14.04
 C       1.533888     0.082347     0.476817      63.05
 H       1.840405     0.882093     1.195021      18.18
 C       0.157437    -0.157018     0.546906      21.56
 O      -0.689225     0.245447     1.581189     225.35
 C      -0.082539     0.887399     2.712308     115.75
 H      -0.875638     1.225048     3.333902      25.77
 H       0.502001     0.179141     3.437938      24.78
 H       0.445400     1.774275     2.396486      23.99
 C      -0.495547    -1.045744    -0.361802      15.76
 O      -1.876646    -1.183925    -0.204675     168.85
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 C       0.259435    -1.711898    -1.387316      90.96
 H      -0.156341    -2.499345    -2.081178      21.11
 C       2.274702    -0.509039    -0.584748      38.94
 C       3.734365    -0.273554    -0.735125      80.13
 H       3.956906    -0.496701    -1.887850      16.38
 O       3.948085     1.169756    -0.593227     262.95
 H       4.845062     1.302109    -0.914050      21.73
 C       4.715848    -1.060355     0.217435      82.01
 H       4.675862    -0.787869     1.238318      25.75
 O       4.482423    -2.566937     0.173378     328.78
 H       4.518631    -2.806727    -0.832976      26.87
 C       6.178535    -0.912904    -0.367413     104.92
 O       6.748362     0.450822    -0.243345     289.62
 H       7.046954     0.564007     0.837255      23.23
 H       6.179812    -1.077743    -1.468457      31.82
 H       6.807198    -1.662478     0.031288      30.56
55
name= lig-ACN-Water-frame_84
 C      -3.901222     0.066575    -3.417184      31.17
 H      -4.134481    -0.883501    -4.003058      21.12
 C      -3.772076     1.429650    -1.419903      67.63
 H      -3.933549     1.467572    -0.371043      21.85
 C      -3.687577     2.634858    -2.160344      14.44
 O      -3.591271     3.927855    -1.606567     207.89
 C      -3.562229     4.079210    -0.176609     113.05
 H      -2.582849     3.606016     0.246475      27.03
 H      -4.446279     3.578938     0.320223      27.26
 H      -3.666617     5.128826     0.001664      26.91
 C      -3.859454     2.530045    -3.562395      13.59
 O      -4.039165     3.673340    -4.395046      29.02
 H      -4.335971     4.401598    -3.840101      22.57
 C      -3.904724     1.284351    -4.183560      49.47
 H      -4.135364     1.409261    -5.261930      30.91
 C      -3.857773     0.176362    -2.010370      29.74
 C      -4.000073    -1.162377    -1.283473      79.28
 H      -4.699631    -1.732080    -1.892098      24.01
 O      -4.814048    -1.070073    -0.033480     193.21
 H      -4.258067    -0.730096     0.646758      26.23
 C      -2.699243    -1.961656    -1.082767      99.05
 H      -2.165097    -2.099852    -1.998275      25.72
 C      -2.814466    -3.395087    -0.483559     108.49
 O      -3.488596    -4.287198    -1.430097     238.72
 H      -2.806123    -4.567231    -2.050452      31.08
 H      -3.399199    -3.317149     0.453174      25.38
 H      -1.677118    -3.646580    -0.322781      24.33
 C       1.608600    -1.332149    -1.504169      36.60
 H       2.071022    -1.811299    -2.380728      22.01
 C       1.507685     0.135415     0.457630      61.19
 H       2.167004     0.709608     1.047673      23.00
 C       0.102205    -0.164252     0.563723      13.31
 O      -0.703738     0.273826     1.582789     211.17
 C      -0.124762     0.940122     2.722858     100.94
 H      -0.995650     1.164253     3.318224      25.22
 H       0.605520     0.161264     3.215586      24.60
 H       0.497118     1.838761     2.528448      25.54
 C      -0.503454    -1.100590    -0.377401      20.33
 O      -1.866047    -1.202460    -0.172516     184.13
 C       0.264144    -1.681879    -1.388900      54.12
 H      -0.180132    -2.396690    -2.044595      19.22
 C       2.232392    -0.495271    -0.599986      39.39
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 C       3.748304    -0.292449    -0.739930     100.17
 H       4.139130    -0.678936    -1.788439      22.17
 O       3.997973     1.116570    -0.538118     273.85
 H       4.925318     1.338387    -0.682350      21.37
 C       4.742812    -1.100043     0.180549      91.58
 H       4.591793    -0.731701     1.152792      26.93
 O       4.493926    -2.541608     0.182842     326.36
 H       4.545713    -2.835878    -0.750191      29.04
 C       6.193869    -0.866368    -0.334686     101.38
 O       6.701170     0.441035    -0.230943     351.97
 H       7.124292     0.601959     0.798726      22.51
 H       6.184953    -1.126051    -1.431412      29.82
 H       6.807529    -1.540078     0.223771      29.07
55
name= lig-ACN-Water-frame_85
 C      -3.967430     0.156626    -3.462755      48.86
 H      -3.946750    -0.925337    -3.841295      29.51
 C      -3.768523     1.455107    -1.372282      64.18
 H      -3.759462     1.517862    -0.255852      25.76
 C      -3.717627     2.597765    -2.190686       7.51
 O      -3.683173     3.865187    -1.653580     220.92
 C      -3.568807     4.050182    -0.217113     109.77
 H      -2.553395     3.623977     0.227499      27.41
 H      -4.403444     3.577876     0.314587      27.57
 H      -3.534972     5.174344    -0.032746      26.77
 C      -3.864172     2.602838    -3.661191      10.62
 O      -4.054363     3.711434    -4.407102     112.11
 H      -4.264314     4.492180    -3.875515      22.36
 C      -3.882235     1.297464    -4.276838      59.42
 H      -4.125199     1.110156    -5.308837      22.09
 C      -3.857851     0.175710    -2.045982      17.31
 C      -4.012686    -1.150564    -1.281880      68.58
 H      -4.576553    -1.779292    -1.903738      24.98
 O      -4.841682    -1.026132    -0.044416     139.17
 H      -4.391299    -0.524126     0.697631      24.44
 C      -2.672725    -1.968061    -1.080759      90.26
 H      -2.256188    -1.940159    -2.096524      27.91
 C      -2.834875    -3.390222    -0.507085     118.68
 O      -3.530331    -4.331260    -1.392057     211.96
 H      -2.823692    -4.561636    -2.039925      29.36
 H      -3.361169    -3.439890     0.463891      26.20
 H      -1.821433    -3.925972    -0.272733      24.05
 C       1.572290    -1.353716    -1.521035      53.00
 H       2.202114    -1.838453    -2.287515      25.79
 C       1.481648     0.120505     0.405121      65.31
 H       1.742107     0.698571     1.199281      24.30
 C       0.149882    -0.211318     0.586166      15.30
 O      -0.747150     0.319767     1.545090     198.82
 C      -0.133837     0.962914     2.770729      99.16
 H      -0.889219     1.184712     3.569945      25.17
 H       0.648278     0.283086     3.288007      25.37
 H       0.284895     1.933032     2.375773      25.39
 C      -0.506781    -1.045293    -0.327007      21.85
 O      -1.877040    -1.210094    -0.109692     149.40
 C       0.196852    -1.655398    -1.401705      68.02
 H      -0.252161    -2.219919    -2.135248      23.61
 C       2.265484    -0.493174    -0.610379      33.82
 C       3.761140    -0.319756    -0.767551      99.04
 H       3.879346    -0.450057    -1.913532      19.62
 O       4.072855     1.111435    -0.488584     260.97
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 H       5.115765     1.100432    -0.420836      13.96
 C       4.726049    -1.138439     0.127641     102.42
 H       4.600204    -0.820089     1.126126      25.54
 O       4.486041    -2.506213     0.191474     346.05
 H       4.610944    -2.887284    -0.680712      30.02
 C       6.221446    -0.917121    -0.271780      97.80
 O       6.672818     0.507044    -0.238047     346.40
 H       7.089495     0.739989     0.782675      23.01
 H       6.375251    -1.229349    -1.350387      29.89
 H       6.888325    -1.592584     0.271931      29.73
55
name= lig-ACN-Water-frame_86
 C      -3.949855     0.197608    -3.459929      44.97
 H      -4.008265    -0.685271    -4.112702      19.27
 C      -3.747398     1.420125    -1.431097      64.39
 H      -3.500260     1.551325    -0.313782      22.87
 C      -3.785679     2.587372    -2.235270      15.43
 O      -3.752369     3.856791    -1.680791     214.16
 C      -3.574787     4.010185    -0.258674     106.87
 H      -2.569150     3.485232     0.135954      24.59
 H      -4.402981     3.680905     0.331174      25.63
 H      -3.544564     5.194282    -0.187757      24.74
 C      -3.869163     2.554335    -3.657158      12.54
 O      -4.041392     3.755090    -4.451398      86.16
 H      -4.399129     4.474051    -3.922446      24.64
 C      -3.933693     1.335727    -4.317645      50.10
 H      -4.050869     1.407626    -5.363535      30.89
 C      -3.890099     0.188674    -2.040399      15.71
 C      -4.068111    -1.160321    -1.228352      72.12
 H      -4.687421    -1.821763    -1.757089      24.25
 O      -4.835557    -0.974485    -0.080765     161.29
 H      -4.359425    -0.321431     0.623419      22.17
 C      -2.697179    -1.916063    -1.054201      92.44
 H      -2.134953    -2.004399    -2.028402      24.83
 C      -2.861045    -3.443352    -0.503100     110.92
 O      -3.580790    -4.351694    -1.365503     203.26
 H      -2.908946    -4.808915    -1.991820      28.11
 H      -3.516935    -3.254320     0.357092      25.63
 H      -1.794362    -3.728057    -0.208915      25.03
 C       1.597283    -1.386749    -1.512528      45.73
 H       2.166575    -1.905623    -2.293874      19.17
 C       1.501803     0.103921     0.463755      61.65
 H       2.117851     0.840036     0.884684      18.92
 C       0.095193    -0.216588     0.631277      12.35
 O      -0.736654     0.371845     1.572259     210.75
 C      -0.133565     0.976214     2.738340     100.97
 H      -1.092473     0.995469     3.382323      23.01
 H       0.705161     0.350075     3.149784      25.31
 H       0.297575     2.038269     2.605775      24.22
 C      -0.566365    -1.048649    -0.336564      21.00
 O      -1.908922    -1.223560    -0.058329     179.89
 C       0.165173    -1.592903    -1.416964      66.14
 H      -0.314609    -2.225534    -2.108542      22.45
 C       2.249558    -0.533945    -0.611005      52.23
 C       3.765045    -0.228377    -0.831162     110.34
 H       4.143997    -0.491000    -1.863447      17.59
 O       4.144258     1.090680    -0.439904     261.51
 H       5.220915     1.144400    -0.444028      11.51
 C       4.735355    -1.105366     0.120073      84.52
 H       4.555630    -0.683531     1.090788      21.99
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 O       4.450836    -2.587303     0.174596     355.17
 H       4.586836    -2.883528    -0.778983      28.02
 C       6.278954    -0.927816    -0.257625      91.44
 O       6.638895     0.529361    -0.260560     382.82
 H       7.008726     0.743194     0.763976      25.97
 H       6.481693    -1.288236    -1.302447      29.39
 H       6.872325    -1.431562     0.544871      29.25
55
name= lig-ACN-Water-frame_87
 C      -3.941279     0.124498    -3.544279      47.63
 H      -4.204210    -0.811405    -3.913983      23.34
 C      -3.710600     1.421113    -1.512706      58.83
 H      -3.649410     1.452203    -0.364645      17.99
 C      -3.829533     2.616152    -2.237616      23.87
 O      -3.796580     3.869250    -1.693942     269.87
 C      -3.589939     4.011288    -0.300486     108.67
 H      -2.605735     3.422648     0.042870      23.24
 H      -4.415835     3.628585     0.238682      25.27
 H      -3.377951     5.170904    -0.002878      23.46
 C      -3.947331     2.652108    -3.667731      27.34
 O      -4.010266     3.727798    -4.451013     111.31
 H      -4.249983     4.519362    -3.884182      22.04
 C      -3.980998     1.387157    -4.261035      46.60
 H      -4.105504     1.288426    -5.319251      25.83
 C      -3.925294     0.130704    -2.118539       4.16
 C      -4.067027    -1.156898    -1.306429      95.87
 H      -4.645696    -1.785162    -1.939489      29.28
 O      -4.847394    -0.899296    -0.034524     172.43
 H      -4.215085    -0.507303     0.684953      22.83
 C      -2.769510    -1.967796    -1.019916      91.57
 H      -2.271899    -1.884247    -2.064257      26.29
 C      -2.934612    -3.363688    -0.461702     121.32
 O      -3.618004    -4.371090    -1.353279     201.65
 H      -2.863784    -4.740849    -1.868925      30.43
 H      -3.480154    -3.426673     0.489496      25.70
 H      -1.967838    -3.844783    -0.219779      25.51
 C       1.559456    -1.414035    -1.484413      23.74
 H       2.011585    -1.892618    -2.350386      14.91
 C       1.525570     0.055045     0.450679      69.07
 H       1.882393     0.824962     1.170280      15.01
 C       0.141708    -0.155003     0.611163      27.43
 O      -0.713356     0.413228     1.566815     233.06
 C      -0.145882     0.984673     2.763722     103.36
 H      -0.866502     1.047066     3.683219      23.17
 H       0.654506     0.323864     3.116976      25.35
 H       0.236631     2.038914     2.527812      22.67
 C      -0.546428    -1.029107    -0.308040      18.58
 O      -1.961301    -1.232671    -0.043246     173.78
 C       0.188860    -1.568611    -1.403241      93.14
 H      -0.267181    -2.281358    -2.123765      22.60
 C       2.261106    -0.534829    -0.607115      31.73
 C       3.822685    -0.261878    -0.799584      80.24
 H       3.926684    -0.339734    -1.890735      18.67
 O       4.151182     1.146333    -0.437395     246.31
 H       5.211373     1.167253    -0.436357      13.83
 C       4.744191    -1.174188     0.097356      82.79
 H       4.549630    -0.885653     1.142830      24.25
 O       4.430629    -2.581530     0.123704     362.15
 H       4.584540    -2.961228    -0.847929      28.25
 C       6.256380    -0.884313    -0.219651      94.80
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 O       6.620624     0.504288    -0.306095     398.17
 H       7.129484     0.802153     0.586560      29.12
 H       6.547806    -1.418144    -1.156141      30.46
 H       6.924468    -1.406773     0.551537      29.36
55
name= lig-ACN-Water-frame_88
 C      -4.022825     0.103617    -3.587089      69.50
 H      -4.128208    -0.646050    -4.279068      24.02
 C      -3.753301     1.393776    -1.555828      65.13
 H      -3.784169     1.406609    -0.452183      22.88
 C      -3.837043     2.644372    -2.234723       5.65
 O      -3.811105     3.937237    -1.700337     213.57
 C      -3.579699     3.989784    -0.263539     108.22
 H      -2.640639     3.354926     0.071653      24.92
 H      -4.427533     3.668613     0.312995      26.58
 H      -3.467377     5.188160    -0.113827      24.36
 C      -4.008709     2.579714    -3.637190      -4.90
 O      -3.990902     3.776394    -4.458251      28.14
 H      -4.416739     4.593409    -3.885623      21.91
 C      -4.029353     1.294243    -4.267748      33.86
 H      -4.209596     1.385536    -5.364798      23.04
 C      -3.871161     0.143405    -2.201558      28.68
 C      -4.113788    -1.132832    -1.300230      72.05
 H      -4.794415    -1.846852    -1.745768      24.04
 O      -4.822074    -0.854845    -0.049167     188.37
 H      -4.210589    -0.579476     0.601758      27.51
 C      -2.805514    -1.945593    -1.040853      83.18
 H      -2.236525    -2.289376    -1.992628      23.75
 C      -3.020169    -3.407210    -0.402257     115.36
 O      -3.629689    -4.341990    -1.329929     205.13
 H      -2.956698    -4.604254    -1.960976      30.37
 H      -3.605867    -3.283367     0.524876      25.65
 H      -2.001350    -3.644625    -0.190458      26.32
 C       1.593529    -1.355739    -1.483346      24.05
 H       2.189729    -1.809458    -2.268386      17.17
 C       1.524430     0.068796     0.464954      80.36
 H       2.160472     0.581770     1.306691      19.78
 C       0.108966    -0.138172     0.564987      19.56
 O      -0.712865     0.441489     1.554145     211.02
 C      -0.062876     0.994318     2.821998      92.67
 H      -1.017958     1.042345     3.466939      22.37
 H       0.770825     0.435973     3.211707      25.32
 H       0.289248     2.040571     2.612304      23.87
 C      -0.596880    -1.012565    -0.291226      22.99
 O      -1.938183    -1.216108    -0.058413     183.75
 C       0.142046    -1.616201    -1.322729      69.13
 H      -0.410166    -2.249374    -2.117158      15.59
 C       2.320607    -0.534222    -0.578539      81.32
 C       3.784859    -0.283500    -0.752576      95.81
 H       4.119174    -0.517554    -1.744088      20.13
 O       4.095239     1.167871    -0.469807     269.89
 H       5.082947     1.168654    -0.337442      15.36
 C       4.732845    -1.188704     0.112713      98.00
 H       4.524539    -0.864180     1.176956      21.81
 O       4.433028    -2.575828     0.026290     352.67
 H       4.614469    -2.923274    -0.960461      28.18
 C       6.248509    -0.957063    -0.183861      96.17
 O       6.645070     0.489646    -0.378651     365.79
 H       6.921823     0.792355     0.527116      31.30
 H       6.461262    -1.352224    -1.185349      31.32
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 H       6.866190    -1.430813     0.662451      29.44
55
name= lig-ACN-Water-frame_89
 C      -4.087189     0.084000    -3.645475      36.01
 H      -4.082661    -0.913166    -4.012366      39.66
 C      -3.841938     1.405545    -1.540729      62.86
 H      -3.715386     1.418481    -0.497301      29.07
 C      -3.850769     2.630072    -2.259111      -7.59
 O      -3.792806     3.924725    -1.672271     182.93
 C      -3.585199     4.013319    -0.226632     108.70
 H      -2.630249     3.433895     0.089287      26.96
 H      -4.460920     3.627596     0.322241      26.23
 H      -3.365146     5.138716     0.068777      24.77
 C      -4.008842     2.599168    -3.695525      18.36
 O      -4.009822     3.741001    -4.412663      57.14
 H      -4.427998     4.602016    -3.879464      19.00
 C      -4.114348     1.373479    -4.375756      60.74
 H      -4.200428     1.336776    -5.524167      17.98
 C      -3.890242     0.115597    -2.189755     -39.24
 C      -4.093020    -1.133460    -1.286701      72.84
 H      -4.730302    -1.766702    -1.948996      23.04
 O      -4.771645    -0.817628    -0.075005     164.71
 H      -4.263982    -0.182877     0.478999      25.66
 C      -2.806251    -1.992607    -1.011201      87.86
 H      -2.306147    -1.923972    -2.054551      27.24
 C      -3.047047    -3.369355    -0.345524     120.42
 O      -3.649259    -4.302393    -1.304494     168.91
 H      -2.918111    -4.542218    -1.967418      28.33
 H      -3.855311    -3.370589     0.414669      25.29
 H      -2.221790    -3.813520     0.108824      27.26
 C       1.552704    -1.323760    -1.469640      55.62
 H       1.982164    -1.832057    -2.324707      23.12
 C       1.508421     0.051774     0.507805      58.31
 H       2.065256     0.789500     1.277272      17.73
 C       0.113055    -0.099758     0.612009      17.25
 O      -0.655892     0.478274     1.598055     229.40
 C      -0.044901     1.007602     2.792650     111.57
 H      -0.845592     1.064931     3.582037      24.91
 H       0.632255     0.255610     3.154007      27.34
 H       0.401854     1.994814     2.678065      25.53
 C      -0.584223    -1.003428    -0.343905      14.80
 O      -1.977468    -1.195894    -0.109449     150.67
 C       0.237219    -1.646326    -1.299581      52.25
 H      -0.218376    -2.393315    -2.071881      20.17
 C       2.231187    -0.535623    -0.542306      49.51
 C       3.798069    -0.267179    -0.734781      83.18
 H       3.957554    -0.494458    -1.749965      20.60
 O       4.014346     1.102376    -0.491766     310.93
 H       4.932543     1.251111    -0.608205      21.85
 C       4.716330    -1.140590     0.188641      91.88
 H       4.520129    -0.989697     1.311889      22.68
 O       4.436740    -2.592002    -0.051809     383.10
 H       4.553983    -2.813306    -1.067818      24.44
 C       6.237697    -0.979689    -0.218802     101.01
 O       6.662491     0.427301    -0.404735     355.74
 H       7.087379     0.759028     0.371665      33.06
 H       6.432069    -1.595955    -1.098053      33.71
 H       6.929488    -1.461975     0.557687      29.15
55
name= lig-ACN-Water-frame_90
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 C      -4.086755     0.198363    -3.593945      61.12
 H      -4.333855    -0.681887    -4.276235      10.74
 C      -3.882949     1.414974    -1.544965      75.01
 H      -3.743800     1.501526    -0.530293      24.98
 C      -3.887099     2.603669    -2.258638      11.11
 O      -3.754700     3.856806    -1.656352     220.30
 C      -3.569266     4.005814    -0.210358     108.08
 H      -2.675860     3.428042     0.160610      27.37
 H      -4.479440     3.621821     0.375416      25.07
 H      -3.507833     5.123035    -0.070294      24.91
 C      -3.999943     2.591091    -3.697828      10.19
 O      -4.058395     3.778579    -4.415665     105.77
 H      -4.058074     4.567031    -3.772790      18.83
 C      -4.161237     1.339498    -4.381578       9.74
 H      -4.234790     1.364511    -5.537012      29.72
 C      -3.988386     0.172480    -2.214956      33.16
 C      -4.029864    -1.137846    -1.334053      65.97
 H      -4.729329    -1.960067    -1.712778      26.79
 O      -4.761382    -0.794747    -0.079066      97.68
 H      -4.248063    -0.063870     0.504837      24.51
 C      -2.745278    -1.962732    -1.006589      90.92
 H      -2.222494    -2.375502    -1.944473      26.69
 C      -3.125923    -3.339180    -0.313323     122.47
 O      -3.652024    -4.277836    -1.314374     141.82
 H      -2.860872    -4.616801    -1.854299      27.69
 H      -3.851872    -3.021461     0.448551      27.26
 H      -2.261194    -3.661665     0.153524      28.31
 C       1.595181    -1.356777    -1.461733      43.72
 H       2.270755    -1.731983    -2.234466      17.64
 C       1.482261     0.065674     0.546576      58.43
 H       1.919745     0.894389     1.267031      18.18
 C       0.090133    -0.141737     0.629541      15.90
 O      -0.682967     0.515531     1.608157     228.68
 C      -0.000203     0.978960     2.816553     115.75
 H      -0.775198     1.232510     3.508605      26.37
 H       0.752540     0.300398     3.217223      28.61
 H       0.520975     1.869253     2.552687      26.96
 C      -0.563538    -0.974598    -0.293501      12.94
 O      -1.955466    -1.133543    -0.137668     157.86
 C       0.165428    -1.665953    -1.313427      70.98
 H      -0.276701    -2.509969    -1.934909      21.85
 C       2.250141    -0.512113    -0.522616      45.88
 C       3.697526    -0.334337    -0.716079     113.65
 H       3.973235    -0.575555    -1.681455      22.89
 O       3.961726     1.119188    -0.485173     273.33
 H       4.902792     1.202049    -0.771077      22.56
 C       4.717502    -1.219250     0.137947      88.65
 H       4.496653    -0.948445     1.247894      25.55
 O       4.422079    -2.558285    -0.040380     362.27
 H       4.627046    -2.838266    -0.996239      29.13
 C       6.219990    -0.980795    -0.208200     101.94
 O       6.690529     0.353600    -0.435918     354.34
 H       6.975664     0.616174     0.450011      30.38
 H       6.323009    -1.394898    -1.205566      33.22
 H       6.839829    -1.512714     0.568398      29.42
55
name= lig-ACN-Water-frame_91
 C      -4.152725     0.175845    -3.613457      44.96
 H      -4.321599    -0.853139    -4.104552      31.19
 C      -3.890140     1.400839    -1.526450      68.09
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 H      -3.887667     1.411132    -0.460145      20.97
 C      -3.902296     2.607572    -2.265252       4.04
 O      -3.708356     3.813611    -1.668985     194.09
 C      -3.575568     3.974166    -0.228294     110.07
 H      -2.649381     3.569249     0.186879      27.80
 H      -4.517435     3.592234     0.362513      24.56
 H      -3.498599     5.028221    -0.124237      26.20
 C      -4.023379     2.650730    -3.682344      32.47
 O      -4.086850     3.821441    -4.422544      27.31
 H      -4.121365     4.553382    -3.871275      26.75
 C      -4.122079     1.437146    -4.315019      26.06
 H      -4.322331     1.369575    -5.420319      20.54
 C      -4.047939     0.159135    -2.185172     -15.44
 C      -4.050159    -1.105811    -1.339271      67.36
 H      -4.702376    -1.834907    -1.987707      25.44
 O      -4.747819    -0.807213    -0.096291     159.43
 H      -4.103016    -0.455191     0.590533      24.45
 C      -2.712240    -1.926976    -1.033852      89.70
 H      -2.129072    -2.086576    -1.960597      27.96
 C      -3.156812    -3.242201    -0.295318     113.48
 O      -3.642454    -4.240643    -1.297800     153.81
 H      -2.884755    -4.630516    -1.730001      30.41
 H      -4.005074    -3.278436     0.387294      25.65
 H      -2.341225    -3.684693     0.193699      27.73
 C       1.558572    -1.407365    -1.385227      66.56
 H       2.075326    -2.020566    -2.137560      22.56
 C       1.468415     0.095090     0.530175      67.71
 H       2.113710     0.667235     1.244438      21.04
 C       0.085977    -0.140247     0.677852       6.01
 O      -0.741371     0.494911     1.597877     212.78
 C       0.055624     1.008736     2.823468     114.01
 H      -0.703189     1.244178     3.479048      26.14
 H       0.606952     0.156327     3.241765      27.63
 H       0.603129     1.869002     2.587713      27.13
 C      -0.564280    -1.043130    -0.291561      18.68
 O      -1.907866    -1.060383    -0.138040     156.53
 C       0.190897    -1.635368    -1.297462      79.96
 H      -0.335369    -2.267927    -1.988533      26.01
 C       2.181461    -0.551860    -0.491611      40.10
 C       3.709893    -0.316545    -0.726966      98.39
 H       3.836893    -0.516908    -1.725299      23.41
 O       3.964568     1.135969    -0.477002     242.93
 H       5.020984     1.227918    -0.545724      17.09
 C       4.665516    -1.175136     0.112832      94.88
 H       4.541512    -0.949778     1.240571      24.05
 O       4.389471    -2.623877     0.005536     367.68
 H       4.624752    -2.918644    -0.896833      28.36
 C       6.184479    -1.048246    -0.279779     104.18
 O       6.710040     0.338390    -0.407061     343.84
 H       7.039387     0.850008     0.426286      26.99
 H       6.391816    -1.584517    -1.201598      31.53
 H       6.773956    -1.619116     0.458258      30.22
55
name= lig-ACN-Water-frame_92
 C      -4.208048     0.155329    -3.581879      71.01
 H      -4.216871    -0.782601    -4.204038      30.90
 C      -3.921507     1.398325    -1.529818      77.57
 H      -3.854246     1.456502    -0.408603      25.96
 C      -3.871673     2.612417    -2.215967       9.71
 O      -3.662007     3.866901    -1.668213     207.53
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 C      -3.568083     3.977761    -0.244070     118.39
 H      -2.726790     3.428258     0.096306      30.36
 H      -4.488725     3.421716     0.271659      26.51
 H      -3.572779     4.960401     0.002529      28.27
 C      -4.048428     2.701772    -3.642572      -1.90
 O      -4.098155     3.860288    -4.419746     118.58
 H      -4.537281     4.656440    -3.994443      25.29
 C      -4.114537     1.410362    -4.308743       2.37
 H      -4.179916     1.513001    -5.390275      17.78
 C      -4.026051     0.164236    -2.198580      26.26
 C      -4.086030    -1.094455    -1.347324      76.78
 H      -4.708055    -1.961402    -1.860932      23.19
 O      -4.755637    -0.868047    -0.098192     136.16
 H      -4.108328    -0.684254     0.537777      26.93
 C      -2.784596    -1.816398    -1.023952      91.25
 H      -2.343838    -2.022575    -1.981618      29.42
 C      -3.107368    -3.232283    -0.344125     122.22
 O      -3.614649    -4.194600    -1.283485     166.47
 H      -2.864854    -4.510774    -1.847508      27.54
 H      -3.853526    -2.837492     0.331349      27.37
 H      -2.296790    -3.553790     0.304453      27.86
 C       1.552371    -1.495924    -1.344430      56.91
 H       2.156184    -2.007348    -2.115900      19.04
 C       1.475653     0.087826     0.537565      66.18
 H       1.895413     0.761475     1.218180      20.82
 C       0.092834    -0.137887     0.671683      21.40
 O      -0.717321     0.471300     1.642511     238.00
 C      -0.020449     1.001349     2.781953     123.27
 H      -0.642180     1.354267     3.515904      26.17
 H       0.665117     0.222508     3.173934      27.69
 H       0.598741     1.796243     2.448692      27.19
 C      -0.536518    -0.994153    -0.220279      17.14
 O      -1.969046    -1.036727    -0.143529     157.64
 C       0.136814    -1.650554    -1.293626      74.99
 H      -0.244057    -2.174788    -2.094390      25.19
 C       2.231294    -0.589506    -0.484569      38.56
 C       3.681336    -0.244682    -0.765498     105.72
 H       3.920875    -0.403254    -1.762726      21.91
 O       4.017382     1.131237    -0.453958     269.42
 H       5.055939     1.134146    -0.428959      18.14
 C       4.668279    -1.200793     0.095638      82.04
 H       4.494668    -0.869293     1.171337      24.01
 O       4.347257    -2.666860     0.060464     376.69
 H       4.498118    -2.950190    -0.858507      30.68
 C       6.179633    -1.076519    -0.308586     105.93
 O       6.682305     0.325584    -0.396361     343.52
 H       7.173250     0.405089     0.514726      28.73
 H       6.308479    -1.467079    -1.316259      31.07
 H       6.735413    -1.611411     0.434790      29.81
55
name= lig-ACN-Water-frame_93
 C      -4.161294     0.218155    -3.614800      76.83
 H      -4.321941    -0.677251    -4.193023      32.11
 C      -3.918855     1.440871    -1.516842      36.49
 H      -3.769600     1.353279    -0.371905      25.54
 C      -3.848311     2.697018    -2.230473      -6.82
 O      -3.631896     3.955700    -1.665822     166.07
 C      -3.557456     3.937061    -0.197797     114.45
 H      -2.683820     3.526770     0.179064      30.59
 H      -4.528209     3.453679     0.250409      26.76
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 H      -3.543166     4.922048     0.050583      27.86
 C      -4.072818     2.632324    -3.630124      -3.89
 O      -4.108896     3.867245    -4.402793      45.29
 H      -4.599662     4.626330    -3.808635      21.91
 C      -4.140778     1.425574    -4.306112     130.58
 H      -4.133579     1.348624    -5.338845      24.59
 C      -4.049009     0.180947    -2.194587     -11.30
 C      -4.133336    -1.124277    -1.335534      51.60
 H      -4.770134    -1.891746    -1.962582      22.73
 O      -4.827255    -0.925345    -0.063760     130.21
 H      -4.271539    -0.342707     0.600111      23.41
 C      -2.764333    -1.826374    -1.094639      89.75
 H      -2.217554    -1.931199    -1.978976      27.34
 C      -3.041033    -3.125962    -0.364876     117.78
 O      -3.564049    -4.160478    -1.280786     146.89
 H      -2.855974    -4.433337    -1.973245      27.16
 H      -3.801036    -3.256848     0.379346      25.39
 H      -2.045900    -3.524297    -0.015822      25.61
 C       1.594659    -1.518186    -1.315483      51.52
 H       2.101055    -1.953160    -2.192660      16.75
 C       1.514170     0.072676     0.542918      56.45
 H       2.011891     0.828800     1.005768      18.61
 C       0.096466    -0.141787     0.679457       9.60
 O      -0.703480     0.415746     1.649820     212.71
 C      -0.018817     1.036965     2.783751     112.55
 H      -0.885274     1.286137     3.344706      25.64
 H       0.636151     0.337847     3.321992      27.42
 H       0.470368     1.959323     2.487403      25.71
 C      -0.653489    -0.995381    -0.284772       8.70
 O      -2.021092    -0.986967    -0.122631     153.31
 C       0.128236    -1.670643    -1.241318      70.63
 H      -0.449045    -2.298781    -1.820239      24.48
 C       2.237114    -0.578406    -0.488168      37.90
 C       3.731560    -0.283944    -0.776142      79.14
 H       3.844642    -0.430456    -1.819584      22.14
 O       4.071690     1.135822    -0.404691     263.31
 H       5.028772     1.161876    -0.545322      18.91
 C       4.664964    -1.265917     0.068504      79.59
 H       4.554872    -0.949956     1.126709      25.62
 O       4.309569    -2.623715     0.094879     375.92
 H       4.539332    -3.048070    -0.791758      31.27
 C       6.159247    -1.084859    -0.332876     101.48
 O       6.629818     0.267247    -0.380002     401.88
 H       7.028545     0.805090     0.434452      28.24
 H       6.271892    -1.458576    -1.365672      31.84
 H       6.783781    -1.718974     0.230611      30.83
55
name= lig-ACN-Water-frame_94
 C      -4.110154     0.198228    -3.582234      28.73
 H      -4.288900    -0.724908    -4.041754      15.75
 C      -3.867022     1.498229    -1.532176      67.75
 H      -3.749394     1.605599    -0.403855      21.19
 C      -3.854762     2.698800    -2.224328       3.88
 O      -3.618036     3.975079    -1.639306     220.57
 C      -3.544517     3.970686    -0.151799     110.68
 H      -2.727463     3.423820     0.142129      31.09
 H      -4.433120     3.412894     0.294409      26.57
 H      -3.553392     4.982271     0.178709      26.83
 C      -4.061668     2.725369    -3.655773       5.26
 O      -4.139743     3.817221    -4.357191      16.87
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 H      -4.178319     4.703188    -3.804169      22.99
 C      -4.154281     1.451078    -4.350168      -4.38
 H      -4.376806     1.550310    -5.359784      32.49
 C      -4.102045     0.250280    -2.153158      31.35
 C      -4.170154    -1.068540    -1.347004      88.89
 H      -4.781659    -1.866818    -1.924253      27.40
 O      -4.893238    -0.964325    -0.054645     110.66
 H      -4.480723    -0.146501     0.458738      26.09
 C      -2.803644    -1.781675    -1.086350      98.29
 H      -2.315768    -1.897828    -2.007409      31.96
 C      -2.894551    -3.202520    -0.420189     131.58
 O      -3.508844    -4.141282    -1.317290     190.77
 H      -2.791299    -4.461487    -1.915123      27.82
 H      -3.423688    -2.918609     0.462008      28.77
 H      -1.841484    -3.490492    -0.032883      26.15
 C       1.501988    -1.486064    -1.326793      44.54
 H       2.035610    -2.113803    -2.052505      21.22
 C       1.492319     0.070065     0.507261      63.91
 H       1.915068     0.665262     1.267662      22.82
 C       0.110825    -0.183084     0.625777      19.50
 O      -0.661424     0.362346     1.649545     207.41
 C      -0.067256     1.120072     2.832382     104.23
 H      -0.836261     1.336322     3.623422      24.88
 H       0.670282     0.449362     3.284520      26.89
 H       0.450923     2.064558     2.536620      26.50
 C      -0.612916    -0.931573    -0.278874      22.13
 O      -2.054054    -0.949110    -0.153033     135.43
 C       0.167209    -1.723226    -1.176614      73.74
 H      -0.057068    -2.521013    -1.855643      24.44
 C       2.240121    -0.569168    -0.525421      44.71
 C       3.754665    -0.323916    -0.734977      98.45
 H       4.028675    -0.437671    -1.789275      21.23
 O       4.093288     1.092701    -0.378482     276.02
 H       5.001512     1.157373    -0.643378      23.77
 C       4.687557    -1.222151     0.107134     100.82
 H       4.584583    -0.858960     1.120040      26.10
 O       4.267760    -2.636198     0.089990     352.30
 H       4.522605    -2.954443    -0.880007      26.06
 C       6.160019    -1.148084    -0.379845     109.78
 O       6.586453     0.283008    -0.402830     352.28
 H       6.947858     0.397965     0.499422      30.81
 H       6.255724    -1.489508    -1.428019      32.49
 H       6.753276    -1.712890     0.279490      30.98
55
name= lig-ACN-Water-frame_95
 C      -4.146513     0.267966    -3.550148      75.68
 H      -4.175151    -0.628769    -4.099349      23.26
 C      -3.846297     1.532012    -1.491938      35.00
 H      -3.717679     1.513021    -0.416581      22.67
 C      -3.833264     2.752815    -2.216069     -13.12
 O      -3.632720     3.950255    -1.595861     164.10
 C      -3.529414     3.982427    -0.147331     112.85
 H      -2.656841     3.554409     0.227012      29.86
 H      -4.420524     3.570768     0.306093      26.42
 H      -3.457413     5.089011     0.097302      25.15
 C      -4.014147     2.663854    -3.611678       3.74
 O      -4.177701     3.895834    -4.398617      21.99
 H      -4.053208     4.619882    -3.847356      27.41
 C      -4.158898     1.448488    -4.277857     112.67
 H      -4.316469     1.435304    -5.337210      37.48
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 C      -4.084103     0.289009    -2.142144     -23.04
 C      -4.194492    -1.044279    -1.302769      69.50
 H      -4.771991    -1.756356    -1.961978      25.39
 O      -4.934823    -0.940198    -0.093587     154.08
 H      -4.549757    -0.309913     0.488429      30.26
 C      -2.781477    -1.728677    -1.094971     105.51
 H      -2.350769    -1.696625    -2.070260      32.26
 C      -2.762288    -3.191142    -0.480361     117.36
 O      -3.453846    -4.154312    -1.344625     194.19
 H      -2.862604    -4.604812    -1.948912      30.12
 H      -3.419864    -3.405033     0.357201      25.97
 H      -1.698381    -3.628372    -0.250983      24.70
 C       1.576632    -1.458759    -1.348146      61.27
 H       2.155356    -2.080515    -2.035528      20.95
 C       1.498365     0.057611     0.491683      62.55
 H       2.093007     0.583118     1.287540      22.79
 C       0.111654    -0.118596     0.669170       7.68
 O      -0.632229     0.377655     1.724975     216.44
 C      -0.067075     1.123376     2.817937     100.35
 H      -1.027792     1.254846     3.467238      24.26
 H       0.785466     0.635327     3.311492      26.53
 H       0.203044     2.152365     2.399834      25.62
 C      -0.631037    -0.982652    -0.310593       8.02
 O      -1.985721    -0.903364    -0.212910     145.03
 C       0.120075    -1.789580    -1.170828      61.51
 H      -0.587333    -2.458089    -1.740469      25.71
 C       2.246923    -0.536785    -0.549132      40.73
 C       3.737583    -0.297113    -0.706033      90.72
 H       3.926506    -0.587434    -1.775599      23.01
 O       4.065243     1.056817    -0.379601     258.14
 H       5.095008     1.075992    -0.433972      19.92
 C       4.686141    -1.253901     0.154109     100.87
 H       4.705132    -0.982196     1.174666      27.68
 O       4.255712    -2.626735     0.083697     367.15
 H       4.402350    -2.941848    -0.924177      25.15
 C       6.148301    -1.141474    -0.387581     106.96
 O       6.587749     0.252611    -0.431951     326.04
 H       7.133476     0.642396     0.219329      33.27
 H       6.253878    -1.545992    -1.419944      32.53
 H       6.794233    -1.721121     0.242527      30.97
55
name= lig-ACN-Water-frame_96
 C      -4.206319     0.263472    -3.496618      95.99
 H      -4.344159    -0.693166    -4.013587      31.71
 C      -3.857775     1.514444    -1.437304      76.65
 H      -3.729529     1.576343    -0.421360      26.26
 C      -3.793706     2.713826    -2.170936      -1.26
 O      -3.647724     3.972958    -1.581519     203.49
 C      -3.508200     4.041481    -0.130807     112.10
 H      -2.649330     3.487188     0.214472      30.60
 H      -4.326433     3.677215     0.381932      29.14
 H      -3.438006     5.199797     0.051548      24.77
 C      -4.010242     2.808727    -3.633255      11.78
 O      -4.176349     3.870064    -4.398499      78.36
 H      -4.433396     4.743615    -3.984580      21.32
 C      -4.148754     1.507096    -4.222779      10.37
 H      -4.248932     1.493180    -5.354533      21.05
 C      -4.027278     0.272702    -2.083897      17.57
 C      -4.134753    -1.036402    -1.314626      63.62
 H      -4.695683    -1.756725    -1.914016      23.53
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 O      -4.987765    -0.896676    -0.108583     162.21
 H      -4.433444    -0.424526     0.540974      27.71
 C      -2.744099    -1.733012    -1.110061      81.27
 H      -2.296218    -1.813120    -2.100833      27.52
 C      -2.748874    -3.206396    -0.557742     121.52
 O      -3.421826    -4.191379    -1.410701     213.71
 H      -2.712924    -4.467277    -2.076615      26.81
 H      -3.009580    -3.098113     0.492412      26.48
 H      -1.595138    -3.390925    -0.518561      23.74
 C       1.533435    -1.544001    -1.384199      44.86
 H       2.057650    -1.931571    -2.249230      17.00
 C       1.511685     0.074135     0.553003      56.25
 H       2.080269     0.870201     1.196859      18.61
 C       0.129481    -0.108988     0.672042      20.78
 O      -0.640485     0.339322     1.736262     211.19
 C      -0.069728     1.179016     2.785720     110.09
 H      -0.871891     1.212697     3.672456      24.82
 H       0.798657     0.664923     3.264438      26.14
 H       0.212971     2.260297     2.495607      24.93
 C      -0.524314    -0.955996    -0.229231      12.67
 O      -1.950728    -0.845393    -0.250681     127.32
 C       0.188075    -1.728923    -1.205564      56.21
 H      -0.172654    -2.473444    -2.028492      22.38
 C       2.186874    -0.554036    -0.544351      31.32
 C       3.718602    -0.331846    -0.685513      86.01
 H       4.022984    -0.409745    -1.782177      19.43
 O       4.038695     1.086998    -0.390460     241.11
 H       5.085218     1.082445    -0.309213      18.30
 C       4.661882    -1.284781     0.160999      82.46
 H       4.533084    -0.992998     1.162712      28.00
 O       4.248327    -2.631585     0.109695     390.90
 H       4.518223    -3.010988    -0.841288      28.28
 C       6.157291    -1.122668    -0.328515     101.48
 O       6.637674     0.271843    -0.498701     336.30
 H       7.022916     0.439014     0.386006      32.32
 H       6.168690    -1.481976    -1.375702      32.00
 H       6.829406    -1.766658     0.285476      30.19
55
name= lig-ACN-Water-frame_97
 C      -4.216994     0.327224    -3.453115      51.43
 H      -4.584937    -0.587319    -4.013577      28.21
 C      -3.833972     1.527220    -1.424680      65.79
 H      -3.827779     1.603049    -0.377191      26.52
 C      -3.796927     2.760100    -2.150930       8.49
 O      -3.663058     4.006372    -1.568133     217.58
 C      -3.487294     4.113159    -0.122837     106.17
 H      -2.569860     3.557889     0.195151      30.46
 H      -4.299208     3.778021     0.356975      29.81
 H      -3.282319     5.230347     0.194054      24.97
 C      -4.040007     2.753369    -3.529586      -0.01
 O      -4.161745     3.916539    -4.416291      44.38
 H      -4.586329     4.791918    -3.922259      20.92
 C      -4.150722     1.528730    -4.188125      52.14
 H      -4.481861     1.647079    -5.303966      24.69
 C      -4.015172     0.266980    -2.072771      29.58
 C      -4.101580    -1.073364    -1.316339      74.16
 H      -4.620987    -1.749831    -1.942212      26.59
 O      -4.967488    -0.888805    -0.128725     143.83
 H      -4.426691    -0.457296     0.678086      24.34
 C      -2.715691    -1.732755    -1.146648      96.60
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 H      -2.288241    -1.675082    -2.174576      27.43
 C      -2.666999    -3.177956    -0.622908     116.15
 O      -3.416710    -4.164432    -1.416932     181.99
 H      -2.824192    -4.605714    -2.155138      25.32
 H      -3.199091    -3.394263     0.321689      26.12
 H      -1.616347    -3.610470    -0.562668      23.41
 C       1.618796    -1.474420    -1.351196      64.40
 H       2.094659    -2.042388    -2.139231      21.46
 C       1.545577     0.089417     0.520500      61.09
 H       2.096398     0.896057     1.179311      21.66
 C       0.172130    -0.157615     0.732064      -6.46
 O      -0.682792     0.339092     1.736157     201.44
 C      -0.036226     1.200493     2.800710     102.98
 H      -0.823787     1.278698     3.685564      24.86
 H       0.961892     0.736309     3.065264      24.49
 H       0.142829     2.226567     2.309054      25.23
 C      -0.521477    -0.984264    -0.268918      -4.08
 O      -1.902989    -0.840335    -0.265634     121.54
 C       0.182924    -1.638437    -1.250243      58.17
 H      -0.500655    -2.254163    -1.959473      25.87
 C       2.250027    -0.609632    -0.496992      41.84
 C       3.695783    -0.311435    -0.722559      95.18
 H       3.923775    -0.607133    -1.829524      19.66
 O       4.003207     1.121224    -0.368004     253.30
 H       4.981548     1.176536    -0.562781      19.33
 C       4.622575    -1.208391     0.181803      90.10
 H       4.534238    -0.896415     1.185417      25.71
 O       4.258169    -2.682241     0.166142     338.06
 H       4.440262    -2.987736    -0.807239      26.32
 C       6.128211    -1.108493    -0.320666      98.02
 O       6.696090     0.264817    -0.486279     341.22
 H       7.181760     0.755589     0.318944      28.07
 H       6.270449    -1.614536    -1.290624      30.74
 H       6.804864    -1.612823     0.458834      28.41
55
name= lig-ACN-Water-frame_98
 C      -4.230923     0.332001    -3.476244      63.15
 H      -4.492866    -0.634867    -4.052785      26.39
 C      -3.800241     1.570634    -1.416679      73.38
 H      -3.745944     1.551163    -0.291766      22.36
 C      -3.838520     2.815269    -2.085784     -22.29
 O      -3.671519     4.077764    -1.541842     183.78
 C      -3.447278     4.157314    -0.115437     114.58
 H      -2.541167     3.531628     0.243946      28.11
 H      -4.256529     3.903263     0.438085      27.45
 H      -3.292094     5.274817    -0.045644      24.73
 C      -4.066853     2.813341    -3.552439      34.74
 O      -4.141404     3.887675    -4.337876     -98.84
 H      -4.328087     4.812162    -3.780708      19.65
 C      -4.233247     1.558695    -4.166512      16.92
 H      -4.492594     1.428752    -5.309438      25.55
 C      -4.023557     0.331002    -2.079168       1.85
 C      -4.129303    -1.057946    -1.313545      72.80
 H      -4.671073    -1.722541    -1.891113      29.76
 O      -4.893843    -0.950625    -0.132449     186.93
 H      -4.357387    -0.429360     0.512469      28.37
 C      -2.651612    -1.700453    -1.165494      95.17
 H      -2.257793    -1.654389    -2.230036      30.32
 C      -2.632679    -3.239809    -0.633856     123.81
 O      -3.463059    -4.114221    -1.433557     202.28
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 H      -2.832063    -4.572723    -2.078343      26.39
 H      -3.067728    -3.042476     0.375252      27.64
 H      -1.584117    -3.502277    -0.413818      25.67
 C       1.607332    -1.453347    -1.350386      46.43
 H       2.281548    -2.029463    -1.967292      22.52
 C       1.534073     0.084462     0.530168      56.77
 H       2.140957     0.727255     1.252025      21.90
 C       0.151868    -0.233190     0.748781      17.57
 O      -0.663855     0.368453     1.757921     196.17
 C       0.005021     1.190889     2.714197     112.42
 H      -0.717980     1.187088     3.636195      26.47
 H       0.982731     0.783655     3.164656      25.09
 H       0.106931     2.270207     2.373972      26.02
 C      -0.529716    -0.921929    -0.264623      23.30
 O      -1.910464    -0.896978    -0.262547     131.44
 C       0.211401    -1.577372    -1.311915      67.44
 H      -0.260694    -2.150767    -2.155941      24.10
 C       2.297316    -0.577970    -0.442661      31.91
 C       3.756050    -0.276666    -0.701922      98.25
 H       3.997170    -0.342192    -1.864218      18.51
 O       3.973219     1.114085    -0.400880     302.50
 H       4.878438     1.267167    -0.600303      23.91
 C       4.650043    -1.197166     0.166561     101.38
 H       4.496934    -0.850485     1.183296      24.79
 O       4.291069    -2.625249     0.229652     354.27
 H       4.438728    -2.991671    -0.670304      28.35
 C       6.151055    -1.059791    -0.224195      96.11
 O       6.715091     0.264770    -0.491324     371.42
 H       7.244270     0.439703     0.409514      27.69
 H       6.295893    -1.607151    -1.172033      30.17
 H       6.694127    -1.684520     0.609567      28.29
55
name= lig-ACN-Water-frame_99
 C      -4.248589     0.340105    -3.469631      33.72
 H      -4.295601    -0.675081    -3.996103       9.29
 C      -3.812427     1.614224    -1.425849      42.88
 H      -3.554465     1.741907    -0.313729      19.51
 C      -3.882056     2.831383    -2.124101      11.76
 O      -3.685592     4.112155    -1.540283     214.61
 C      -3.406983     4.248254    -0.098759     109.58
 H      -2.488322     3.560058     0.175734      26.29
 H      -4.254386     3.971136     0.464808      25.78
 H      -3.104614     5.237929     0.171698      25.27
 C      -4.090048     2.781514    -3.492253       3.83
 O      -4.106951     3.917162    -4.275840      31.17
 H      -4.494071     4.830173    -3.884303      15.42
 C      -4.330035     1.557949    -4.178792      15.06
 H      -4.387201     1.775570    -5.312108      38.58
 C      -4.047611     0.342831    -2.069441      27.69
 C      -4.067378    -1.017044    -1.391242      85.16
 H      -4.610297    -1.639071    -2.012796      29.37
 O      -4.809897    -1.023236    -0.069817     128.53
 H      -4.479197    -0.364264     0.493517      28.70
 C      -2.677386    -1.747672    -1.219596      94.29
 H      -2.074569    -1.738438    -2.201189      29.83
 C      -2.672226    -3.148599    -0.614872     121.64
 O      -3.495463    -4.065198    -1.429834     216.76
 H      -2.926154    -4.479826    -2.078619      30.33
 H      -3.106717    -3.276882     0.397687      26.61
 H      -1.737162    -3.626016    -0.666849      27.16
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 C       1.655697    -1.435393    -1.325627      43.08
 H       2.080900    -1.907378    -2.202263      13.05
 C       1.517458     0.030613     0.637972      67.28
 H       1.936007     0.737369     1.314146      20.17
 C       0.155240    -0.186571     0.728262      16.65
 O      -0.610419     0.342050     1.714639     214.88
 C       0.030304     1.213243     2.724913     105.59
 H      -0.671519     1.253773     3.604565      25.77
 H       1.023046     0.697008     2.952129      24.85
 H       0.250051     2.220251     2.303830      26.02
 C      -0.512829    -0.922368    -0.339447      10.02
 O      -1.948215    -0.928578    -0.210174     113.93
 C       0.244765    -1.523120    -1.343972      69.26
 H      -0.178726    -2.117143    -2.116344      28.01
 C       2.254370    -0.540567    -0.473196      46.77
 C       3.779124    -0.273217    -0.695396      73.46
 H       4.036090    -0.594517    -1.822716      20.62
 O       3.977743     1.162278    -0.420795     256.23
 H       4.981147     1.289718    -0.401730      20.73
 C       4.715722    -1.150450     0.217366      83.42
 H       4.539883    -0.776433     1.248622      26.63
 O       4.337023    -2.522547     0.253921     342.87
 H       4.519920    -2.882261    -0.617943      33.36
 C       6.212425    -1.101904    -0.155190      97.74
 O       6.720420     0.247842    -0.449948     369.11
 H       7.134128     0.726441     0.329338      31.91
 H       6.340210    -1.703502    -1.082698      32.08
 H       6.918314    -1.497548     0.691504      28.96
55
name= lig-ACN-Water-frame_100
 C      -4.273800     0.371643    -3.465071      62.79
 H      -4.437512    -0.565347    -4.038659      30.73
 C      -3.841167     1.613174    -1.402610      80.34
 H      -3.569773     1.537425    -0.353858      27.67
 C      -3.889827     2.869247    -2.064114     -20.55
 O      -3.701809     4.129805    -1.559824     141.19
 C      -3.355377     4.264511    -0.108952     109.23
 H      -2.474550     3.552529     0.213958      28.48
 H      -4.240839     4.077771     0.545510      26.46
 H      -3.102825     5.246908    -0.084321      26.48
 C      -4.182691     2.823120    -3.502563      -2.93
 O      -4.069581     3.940640    -4.273157    -156.25
 H      -4.454942     4.799928    -3.919204      13.21
 C      -4.345077     1.593970    -4.168678      74.65
 H      -4.545692     1.526969    -5.254862      24.33
 C      -4.040873     0.383838    -2.071863       7.01
 C      -4.037997    -1.032646    -1.365456      63.69
 H      -4.631145    -1.657067    -1.973771      26.65
 O      -4.716760    -1.091582    -0.079101     131.43
 H      -4.393743    -0.230910     0.424788      27.41
 C      -2.695318    -1.702041    -1.176069      82.44
 H      -2.224829    -1.749115    -2.245533      28.27
 C      -2.751840    -3.168625    -0.650464     129.68
 O      -3.566529    -4.027521    -1.449757     208.90
 H      -2.973925    -4.491072    -2.095104      28.38
 H      -3.131474    -3.119263     0.373476      27.47
 H      -1.742205    -3.355880    -0.546741      28.40
 C       1.657895    -1.371572    -1.393658      33.63
 H       2.338666    -1.729624    -2.171890      16.03
 C       1.598857    -0.017913     0.637155      57.32
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 H       2.109773     0.595615     1.279538      22.05
 C       0.150013    -0.146203     0.638015       6.82
 O      -0.638500     0.340667     1.711487     191.96
 C       0.079724     1.189748     2.708869     116.74
 H      -0.667317     1.352860     3.471125      27.32
 H       0.983495     0.765568     3.242154      26.58
 H       0.265139     2.159676     2.253436      27.08
 C      -0.563896    -0.901798    -0.323075      15.50
 O      -1.912260    -0.954371    -0.201392     143.18
 C       0.214354    -1.539048    -1.351830      66.70
 H      -0.296668    -2.106516    -2.031030      29.00
 C       2.321878    -0.525426    -0.437645      40.00
 C       3.766121    -0.259544    -0.643409      78.46
 H       4.026345    -0.483194    -1.788391      21.98
 O       4.021396     1.203568    -0.438323     225.78
 H       5.066478     1.218602    -0.444331      20.82
 C       4.765426    -1.065334     0.320384      85.81
 H       4.702625    -0.700278     1.398586      25.52
 O       4.370724    -2.477220     0.261941     308.17
 H       4.437472    -2.753884    -0.710958      29.71
 C       6.303661    -1.087542    -0.095527      93.79
 O       6.716201     0.267004    -0.435234     346.51
 H       7.151248     0.551899     0.366319      31.38
 H       6.534499    -1.744871    -0.980888      31.50
 H       6.807488    -1.605008     0.817641      29.45
55
name= lig-ACN-Water-frame_101
 C      -4.320557     0.403945    -3.451041      94.06
 H      -4.619757    -0.499045    -3.937325      31.81
 C      -3.855159     1.607561    -1.360089      78.48
 H      -3.697564     1.700323    -0.342971      27.29
 C      -3.938174     2.841290    -2.084708      -1.38
 O      -3.706374     4.116130    -1.538229     188.85
 C      -3.319855     4.286172    -0.188218     108.15
 H      -2.446782     3.592931     0.102372      30.22
 H      -4.220451     4.129182     0.556896      25.78
 H      -2.979122     5.250162    -0.043178      27.16
 C      -4.216928     2.890724    -3.485364       0.09
 O      -4.042444     3.956102    -4.325247      14.84
 H      -4.221587     4.789872    -3.895698      21.08
 C      -4.362476     1.625170    -4.143776      36.92
 H      -4.654773     1.693936    -5.151143      21.52
 C      -4.036807     0.342476    -2.057855      19.43
 C      -4.072433    -1.010840    -1.339181      78.99
 H      -4.562808    -1.738327    -1.982239      27.49
 O      -4.687414    -1.089484    -0.076036     136.33
 H      -4.294738    -0.436270     0.627803      25.43
 C      -2.665589    -1.680445    -1.189381      89.59
 H      -2.094779    -1.582396    -2.204964      28.28
 C      -2.795102    -3.144582    -0.636130     119.86
 O      -3.625942    -4.030112    -1.507631     132.56
 H      -2.962642    -4.532645    -2.118845      25.65
 H      -3.374131    -3.111683     0.272346      29.09
 H      -1.971498    -3.729294    -0.494191      28.43
 C       1.596749    -1.256864    -1.447722      65.35
 H       2.033280    -1.867469    -2.258200      25.00
 C       1.572006     0.001554     0.615118      63.83
 H       2.079025     0.382233     1.448593      23.30
 C       0.198751    -0.107288     0.673577      17.69
 O      -0.620281     0.356636     1.718219     209.46
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 C       0.042879     1.188768     2.691922     125.03
 H      -0.675460     1.456418     3.395684      28.53
 H       0.825826     0.536073     3.123770      27.02
 H       0.531275     2.047777     2.261630      28.25
 C      -0.478885    -0.895974    -0.340823      11.90
 O      -1.906445    -0.959220    -0.203211     118.58
 C       0.251888    -1.551321    -1.339106      76.93
 H      -0.086829    -2.164890    -2.100823      26.20
 C       2.340677    -0.607188    -0.457470      39.50
 C       3.877643    -0.195392    -0.555874      77.68
 H       4.173994    -0.504481    -1.667251      20.38
 O       4.106153     1.219091    -0.432608     267.03
 H       5.093357     1.276201    -0.537014      21.98
 C       4.806139    -1.088966     0.314193      99.46
 H       4.586983    -0.746698     1.399392      24.15
 O       4.386035    -2.450096     0.290413     333.66
 H       4.489993    -2.812030    -0.690623      25.26
 C       6.281276    -1.037453    -0.037234      96.55
 O       6.761745     0.306407    -0.409570     375.26
 H       7.301822     0.601558     0.322933      31.82
 H       6.356142    -1.723244    -0.935966      30.68
 H       6.981058    -1.323105     0.803561      27.88
55
name= lig-ACN-Water-frame_102
 C      -4.389298     0.410712    -3.406856      27.09
 H      -4.600014    -0.449710    -3.964957      12.85
 C      -3.891047     1.623918    -1.379818      71.68
 H      -3.739199     1.613031    -0.333181      26.21
 C      -3.963316     2.846961    -2.081476       6.64
 O      -3.729962     4.089783    -1.579547     193.60
 C      -3.260671     4.279282    -0.196483     102.95
 H      -2.450938     3.563980     0.043235      28.39
 H      -4.181329     4.071966     0.557204      23.05
 H      -2.938228     5.329156    -0.162464      25.18
 C      -4.141819     2.844408    -3.495805      23.66
 O      -4.024178     3.976895    -4.353432      29.31
 H      -4.490349     4.793371    -4.092943      19.49
 C      -4.437832     1.667687    -4.123459      68.31
 H      -4.532274     1.695870    -5.145295      41.50
 C      -4.082152     0.375630    -2.010860       7.26
 C      -4.014868    -1.028046    -1.359392      41.01
 H      -4.729470    -1.636054    -1.977192      23.11
 O      -4.764207    -1.047271    -0.011910     123.35
 H      -4.131302    -0.665080     0.541500      32.09
 C      -2.599699    -1.718326    -1.219515      78.59
 H      -2.071358    -1.796932    -2.250033      28.89
 C      -2.880618    -3.184385    -0.661903     122.25
 O      -3.649450    -4.024210    -1.573892     160.04
 H      -3.030623    -4.462228    -2.222923      26.79
 H      -3.454060    -3.070042     0.243237      28.59
 H      -1.911414    -3.444275    -0.387259      28.15
 C       1.687059    -1.256248    -1.479650      60.39
 H       2.249749    -1.602687    -2.337620      23.48
 C       1.615154    -0.008124     0.620011      55.43
 H       2.152878     0.554194     1.423654      21.86
 C       0.171325    -0.156571     0.688551      13.71
 O      -0.624280     0.388154     1.675480     222.24
 C       0.056148     1.170800     2.723795     124.33
 H      -0.693024     1.603976     3.292335      28.46
 H       0.695720     0.591105     3.371438      28.56
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 H       0.593044     1.962473     2.260199      28.51
 C      -0.500873    -0.881706    -0.306624      16.40
 O      -1.849267    -0.932686    -0.186612     144.80
 C       0.254826    -1.516451    -1.340116      72.46
 H      -0.358646    -2.162037    -1.976059      28.67
 C       2.382193    -0.510087    -0.463586      40.16
 C       3.906975    -0.263252    -0.609246      82.03
 H       4.223982    -0.518325    -1.706099      18.73
 O       4.221229     1.222292    -0.367247     267.27
 H       5.153657     1.270253    -0.478580      21.49
 C       4.773613    -1.084606     0.391400      85.09
 H       4.662433    -0.776042     1.514222      23.99
 O       4.385782    -2.487121     0.307587     331.44
 H       4.722032    -2.845084    -0.591437      27.73
 C       6.298796    -0.960710    -0.020421     106.93
 O       6.803229     0.363739    -0.423691     408.40
 H       7.346188     0.740983     0.312280      34.47
 H       6.558333    -1.614207    -0.913123      30.78
 H       6.818957    -1.471027     0.812486      28.93
55
name= lig-ACN-Water-frame_103
 C      -4.466348     0.421351    -3.399117     131.52
 H      -4.577784    -0.514760    -3.873805      27.49
 C      -3.931645     1.636210    -1.348490      64.55
 H      -3.702614     1.659026    -0.246085      29.06
 C      -3.920908     2.858491    -2.106527     -14.88
 O      -3.737067     4.124957    -1.582211     176.09
 C      -3.230059     4.224681    -0.235927     109.60
 H      -2.365134     3.653477     0.000278      28.75
 H      -4.122867     4.088541     0.601063      23.52
 H      -2.957694     5.364797    -0.163446      25.05
 C      -4.106481     2.871448    -3.559655      11.09
 O      -4.015510     3.963545    -4.337161     -58.31
 H      -4.492941     4.725715    -3.849290      18.78
 C      -4.479912     1.588914    -4.134940      35.72
 H      -4.669433     1.519065    -5.167518      24.05
 C      -4.144918     0.395377    -2.030232       7.39
 C      -4.043670    -0.985149    -1.306712      59.27
 H      -4.524827    -1.804675    -1.989334      24.07
 O      -4.786753    -1.005766    -0.046098     136.94
 H      -4.327513    -0.645985     0.768848      25.48
 C      -2.693902    -1.744123    -1.173294      90.53
 H      -2.166910    -1.726572    -2.187228      29.68
 C      -2.897794    -3.181637    -0.675563     121.86
 O      -3.619287    -3.999912    -1.643142     196.96
 H      -2.965584    -4.409274    -2.210947      28.63
 H      -3.560353    -3.165304     0.196076      26.95
 H      -2.072829    -3.823761    -0.438598      27.35
 C       1.706999    -1.253273    -1.388197      52.81
 H       2.271725    -1.701394    -2.178420      19.72
 C       1.639725    -0.003566     0.637406      53.47
 H       2.124998     0.770516     1.371052      21.72
 C       0.266502    -0.178744     0.717343       3.61
 O      -0.623953     0.425885     1.670308     193.96
 C       0.054930     1.192034     2.755832     121.28
 H      -0.754082     1.666752     3.244807      27.75
 H       0.574183     0.538610     3.382649      29.13
 H       0.733113     1.917061     2.373273      27.58
 C      -0.436545    -0.914962    -0.311074       8.72
 O      -1.885056    -0.965342    -0.234039     114.79
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 C       0.336835    -1.442710    -1.341505      68.40
 H      -0.006529    -2.112173    -2.216784      26.93
 C       2.376520    -0.404171    -0.521875      37.46
 C       3.886445    -0.230949    -0.602703      86.25
 H       4.207413    -0.504550    -1.664718      22.51
 O       4.293226     1.140582    -0.295934     257.86
 H       5.264509     1.150752    -0.495686      19.73
 C       4.770499    -1.096878     0.364886      66.22
 H       4.466518    -0.676000     1.413070      24.95
 O       4.423167    -2.532795     0.340669     347.00
 H       4.650022    -2.852188    -0.555537      29.86
 C       6.332269    -0.949837    -0.015527     101.40
 O       6.822929     0.412294    -0.431618     323.62
 H       7.425851     0.583976     0.423909      27.02
 H       6.387022    -1.614418    -0.919976      30.94
 H       6.994970    -1.191416     0.786380      28.26
55
name= lig-ACN-Water-frame_104
 C      -4.509702     0.356256    -3.378525       3.14
 H      -4.860370    -0.550599    -3.889944      27.14
 C      -3.951065     1.670414    -1.386390      72.63
 H      -3.785523     1.761026    -0.234488      33.66
 C      -3.874698     2.829553    -2.158404      -6.92
 O      -3.723196     4.149047    -1.590689     182.57
 C      -3.212247     4.234263    -0.259790     108.78
 H      -2.397381     3.580409    -0.172957      31.17
 H      -4.082484     3.803466     0.492920      25.80
 H      -2.876499     5.361048     0.021191      25.15
 C      -4.149266     2.769054    -3.544923       2.27
 O      -4.029778     3.975348    -4.315011      30.07
 H      -4.233409     4.875543    -3.765346      20.07
 C      -4.473713     1.582395    -4.192002      63.51
 H      -4.886996     1.687790    -5.211578      22.03
 C      -4.169865     0.386181    -1.981619      -9.93
 C      -4.130452    -0.963984    -1.263661      51.01
 H      -4.855995    -1.594116    -1.947378      20.92
 O      -4.850344    -0.977007    -0.068052     152.42
 H      -4.235840    -0.390595     0.587263      27.18
 C      -2.720719    -1.689213    -1.140111      78.60
 H      -2.345531    -1.739536    -2.193192      28.45
 C      -2.933144    -3.239673    -0.653162     106.85
 O      -3.602784    -3.970091    -1.741414     210.64
 H      -2.919414    -4.473729    -2.269629      27.11
 H      -3.562388    -3.265926     0.260447      26.04
 H      -1.853521    -3.454379    -0.411511      26.22
 C       1.781948    -1.239258    -1.352248      47.52
 H       2.311865    -1.880175    -2.035706      22.26
 C       1.649404     0.124414     0.633467      51.53
 H       2.242081     0.677344     1.506957      23.55
 C       0.227521    -0.172629     0.740716       1.82
 O      -0.547520     0.455762     1.664956     227.35
 C       0.025623     1.194792     2.773237     124.72
 H      -0.756919     1.729621     3.338888      27.74
 H       0.489893     0.524501     3.389262      30.76
 H       0.743052     1.911200     2.437500      29.53
 C      -0.442580    -0.955052    -0.312248       1.82
 O      -1.840418    -0.984057    -0.242347     146.13
 C       0.366994    -1.448062    -1.371892      62.28
 H      -0.188279    -2.024437    -2.242883      25.81
 C       2.412893    -0.371197    -0.431189      39.90
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 C       3.912860    -0.202403    -0.602748     107.44
 H       4.136603    -0.369885    -1.681374      24.56
 O       4.326710     1.111843    -0.241448     276.00
 H       5.375603     1.117061    -0.334348      16.59
 C       4.770082    -1.142642     0.301978      85.78
 H       4.641833    -0.833102     1.410585      24.93
 O       4.493377    -2.533636     0.378737     324.04
 H       4.466975    -2.855070    -0.537868      29.83
 C       6.308501    -0.958222    -0.028447     106.18
 O       6.836511     0.409676    -0.419406     279.44
 H       7.296949     0.915289     0.428145      25.93
 H       6.628691    -1.588790    -0.882842      30.41
 H       6.811291    -1.407876     0.778598      30.99
55
name= lig-ACN-Water-frame_105
 C      -4.533312     0.382881    -3.398383     104.32
 H      -4.951031    -0.592881    -3.783469      23.19
 C      -3.924742     1.644123    -1.403282      72.26
 H      -3.797881     1.642673    -0.247002      30.07
 C      -3.868867     2.867291    -2.139008     -26.33
 O      -3.698696     4.126244    -1.675554     151.57
 C      -3.189494     4.158878    -0.267444     106.05
 H      -2.268617     3.645606    -0.104106      29.46
 H      -4.050813     3.829913     0.517242      24.32
 H      -3.036863     5.335727    -0.111435      25.01
 C      -4.151077     2.820819    -3.571032     -11.87
 O      -4.059291     3.921976    -4.291990    -146.31
 H      -4.416378     4.747739    -3.723782      21.20
 C      -4.497236     1.540512    -4.146554      32.72
 H      -4.732287     1.457584    -5.277700      23.00
 C      -4.198024     0.405413    -2.037075      -3.98
 C      -4.199578    -0.963245    -1.295222      33.25
 H      -4.702412    -1.829082    -1.952399      23.98
 O      -4.929820    -0.909311     0.039686     128.56
 H      -4.460983    -0.342735     0.696395      29.08
 C      -2.782268    -1.711650    -1.155463      80.85
 H      -2.284329    -1.757405    -2.114882      28.69
 C      -2.934786    -3.173455    -0.709847     114.02
 O      -3.573407    -3.945817    -1.787127     190.84
 H      -2.810494    -4.392461    -2.336656      25.11
 H      -3.556481    -3.327706     0.216132      26.16
 H      -1.941777    -3.760845    -0.514595      24.85
 C       1.795952    -1.259673    -1.349545      16.69
 H       2.497881    -1.543819    -2.129520      17.11
 C       1.604280     0.201425     0.630610      61.79
 H       2.021506     0.791367     1.532099      23.05
 C       0.263270    -0.115114     0.684206      14.83
 O      -0.570233     0.473255     1.671112     208.21
 C       0.054665     1.187528     2.812158     119.59
 H      -0.912082     1.614057     3.218471      25.63
 H       0.565019     0.609454     3.488615      29.32
 H       0.656982     2.012153     2.459369      28.51
 C      -0.406408    -0.911768    -0.299708      14.65
 O      -1.820429    -0.965664    -0.200660     113.17
 C       0.374804    -1.471103    -1.330781      63.37
 H      -0.109462    -2.127892    -2.161704      23.53
 C       2.422853    -0.447330    -0.365116      46.43
 C       3.926611    -0.227637    -0.585672     107.41
 H       4.162996    -0.369584    -1.628215      22.00
 O       4.344610     1.202319    -0.184133     224.48
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 H       5.414340     1.138985    -0.319794      14.99
 C       4.844313    -1.119671     0.297373      95.12
 H       4.661450    -0.647543     1.309948      23.66
 O       4.535062    -2.555587     0.377067     280.57
 H       4.656993    -2.873718    -0.576678      30.19
 C       6.348107    -1.008413    -0.064964     110.59
 O       6.826658     0.374946    -0.375078     371.63
 H       7.302981     0.638371     0.545905      28.17
 H       6.533211    -1.594436    -0.957520      31.92
 H       6.896422    -1.280124     0.786439      29.72
55
name= lig-ACN-Water-frame_106
 C      -4.566599     0.369754    -3.396050      36.81
 H      -4.766991    -0.563197    -4.034302      17.73
 C      -3.881328     1.613084    -1.409466      42.82
 H      -3.556486     1.614055    -0.339617      28.93
 C      -3.916905     2.777399    -2.170713       7.69
 O      -3.614399     4.086984    -1.664018     211.30
 C      -3.199843     4.165362    -0.336448     114.67
 H      -2.278208     3.561159    -0.165626      27.31
 H      -4.065822     3.710452     0.348286      24.64
 H      -2.990519     5.264284    -0.095066      26.23
 C      -4.151187     2.754868    -3.530745      20.10
 O      -4.115412     3.950822    -4.333972     -39.61
 H      -4.454896     4.751692    -3.852788      20.30
 C      -4.503886     1.579709    -4.145039     -34.08
 H      -4.679015     1.622437    -5.314702      32.12
 C      -4.231945     0.359506    -2.027787     -37.35
 C      -4.192394    -0.948998    -1.200837      11.50
 H      -4.958996    -1.646046    -1.777878      15.47
 O      -4.975880    -0.853858     0.080043     145.48
 H      -4.377527    -0.432759     0.654502      32.78
 C      -2.729020    -1.654046    -1.140288      81.99
 H      -2.388450    -1.539790    -2.131202      31.13
 C      -2.928793    -3.176681    -0.771082     108.38
 O      -3.580742    -3.916077    -1.816944     205.31
 H      -2.859349    -4.302952    -2.425056      26.33
 H      -3.638535    -3.146046     0.120276      25.22
 H      -1.841303    -3.549818    -0.434054      24.55
 C       1.776506    -1.244114    -1.312694      67.34
 H       2.173737    -1.680646    -2.244118      22.90
 C       1.648128     0.163328     0.615925      58.27
 H       2.134295     0.959373     1.175868      22.48
 C       0.208597    -0.001924     0.671734       8.80
 O      -0.589124     0.462653     1.682096     227.29
 C       0.016414     1.220605     2.814039     109.81
 H      -0.755586     1.572157     3.572857      25.70
 H       0.677151     0.517662     3.258836      27.98
 H       0.605754     2.084068     2.481943      26.50
 C      -0.419739    -0.868156    -0.329765      -3.50
 O      -1.871494    -0.956632    -0.165631     124.51
 C       0.418464    -1.517157    -1.270853      64.53
 H       0.011356    -2.173667    -2.071347      24.71
 C       2.433413    -0.466682    -0.353504      52.60
 C       3.952234    -0.157842    -0.508581      97.81
 H       4.145110    -0.291342    -1.530789      23.75
 O       4.307474     1.234586    -0.171599     255.35
 H       5.308197     1.320905    -0.399186      20.24
 C       4.912972    -1.098073     0.359111      93.44
 H       4.800154    -0.830898     1.409232      25.16
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 O       4.566266    -2.528786     0.367353     329.11
 H       4.594486    -2.808894    -0.642580      25.95
 C       6.420618    -1.037683    -0.086328      99.40
 O       6.835572     0.322333    -0.303942     363.59
 H       7.552886     0.566659     0.321937      31.43
 H       6.538916    -1.614560    -0.981424      33.30
 H       7.027105    -1.610573     0.590880      29.56
55
name= lig-ACN-Water-frame_107
 C      -4.559306     0.348528    -3.410246      50.44
 H      -4.815786    -0.646966    -3.887281      26.80
 C      -3.848471     1.534048    -1.408488      95.75
 H      -3.467562     1.574006    -0.423453      28.82
 C      -3.877971     2.785879    -2.140422     -33.19
 O      -3.545879     4.008353    -1.723267     171.48
 C      -3.181802     4.139667    -0.318134     116.50
 H      -2.262545     3.500104    -0.069652      28.54
 H      -4.042056     3.826308     0.390834      25.69
 H      -2.948715     5.171307    -0.147749      27.69
 C      -4.213912     2.829228    -3.584014       3.87
 O      -4.179555     3.942128    -4.343942     -64.22
 H      -4.369802     4.700322    -3.820406      27.61
 C      -4.496051     1.562589    -4.182669     -13.22
 H      -4.816216     1.601561    -5.313547      17.03
 C      -4.245562     0.331458    -1.986312      11.37
 C      -4.214502    -0.929753    -1.132085      93.64
 H      -4.683404    -1.804014    -1.767163      27.37
 O      -4.920960    -0.796441     0.089762     177.08
 H      -4.387099    -0.433374     0.905174      25.91
 C      -2.743088    -1.563859    -1.136459      92.72
 H      -2.298321    -1.469656    -2.066447      33.93
 C      -2.914614    -3.111104    -0.782886     110.28
 O      -3.598622    -3.884089    -1.853810     178.64
 H      -2.907446    -4.315612    -2.370715      28.90
 H      -3.546872    -3.269441     0.163687      27.25
 H      -1.873335    -3.664221    -0.533104      25.77
 C       1.800317    -1.293804    -1.313837      43.18
 H       2.539869    -1.861698    -1.915239      21.86
 C       1.635013     0.179989     0.619003      56.90
 H       2.064762     0.808020     1.320074      25.53
 C       0.201349     0.021499     0.639583       5.52
 O      -0.630247     0.515589     1.715229     188.95
 C       0.046481     1.201523     2.791468     113.44
 H      -0.806386     1.337081     3.501871      26.08
 H       0.892043     0.662003     3.273113      27.35
 H       0.354854     2.215441     2.423002      26.58
 C      -0.509442    -0.807869    -0.278765      12.62
 O      -1.874018    -0.951456    -0.153299     149.43
 C       0.329925    -1.525607    -1.207779      59.16
 H      -0.135793    -2.174596    -1.901703      27.20
 C       2.481830    -0.415807    -0.389261      10.51
 C       4.000975    -0.145423    -0.444001      91.04
 H       4.299386    -0.338515    -1.420647      23.33
 O       4.221632     1.257247    -0.185546     282.66
 H       5.153120     1.310406    -0.296066      23.30
 C       4.978248    -1.126999     0.431085      93.24
 H       4.970977    -0.741996     1.418200      26.32
 O       4.560859    -2.468753     0.357557     332.99
 H       4.544552    -2.723028    -0.672280      24.82
 C       6.427631    -1.094900    -0.115184     103.22
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 O       6.917894     0.306255    -0.273441     370.16
 H       7.444849     0.457707     0.507247      30.82
 H       6.450186    -1.450041    -1.106086      32.11
 H       7.043864    -1.630460     0.633666      28.22
55
name= lig-ACN-Water-frame_108
 C      -4.530379     0.346151    -3.381383      73.93
 H      -5.007988    -0.513208    -3.848761      18.87
 C      -3.817621     1.592315    -1.427920      75.25
 H      -3.616769     1.564256    -0.426926      26.27
 C      -3.837894     2.716105    -2.234572     -12.06
 O      -3.453520     3.993268    -1.710147     174.40
 C      -3.141251     4.114251    -0.286691     114.86
 H      -2.247751     3.439767     0.105445      28.83
 H      -4.055042     3.934373     0.295182      27.67
 H      -2.881254     5.099554    -0.215032      29.24
 C      -4.270937     2.738443    -3.570724     -22.39
 O      -4.242261     3.950014    -4.319118     -39.42
 H      -4.580257     4.690456    -3.765903      28.38
 C      -4.510808     1.499759    -4.162187      31.76
 H      -4.743968     1.370477    -5.248828      23.97
 C      -4.247174     0.351399    -2.044892      -5.06
 C      -4.167633    -0.934570    -1.200917      43.75
 H      -4.881757    -1.709054    -1.660167      26.81
 O      -4.851800    -0.769824     0.143494     137.47
 H      -4.096582    -0.291422     0.767497      26.18
 C      -2.767284    -1.583033    -1.103603      93.62
 H      -2.414631    -1.470019    -2.073532      32.36
 C      -2.894794    -3.078545    -0.799463     114.72
 O      -3.607042    -3.821610    -1.862496     198.50
 H      -2.898485    -4.285332    -2.351623      29.85
 H      -3.448649    -3.184372     0.184884      26.92
 H      -1.793224    -3.514793    -0.743874      25.48
 C       1.748846    -1.340911    -1.199501      55.77
 H       2.144665    -2.034244    -1.958715      20.99
 C       1.572369     0.233199     0.613257      61.71
 H       2.017280     0.619756     1.441812      26.40
 C       0.196963     0.023450     0.694513      10.17
 O      -0.585369     0.537524     1.670760     234.00
 C       0.041932     1.246143     2.801020     111.44
 H      -0.640449     1.231957     3.654824      27.17
 H       1.013471     0.685147     3.114269      25.39
 H       0.284650     2.320151     2.545289      26.49
 C      -0.465483    -0.804226    -0.291151       1.61
 O      -1.884897    -0.904138    -0.098622     132.57
 C       0.344242    -1.484956    -1.193238      74.84
 H      -0.069575    -2.211691    -1.780661      27.79
 C       2.409859    -0.408791    -0.391834      19.71
 C       4.011209    -0.218880    -0.442970      99.40
 H       4.276264    -0.394938    -1.423791      24.33
 O       4.170494     1.283668    -0.201335     280.96
 H       5.114992     1.447625    -0.175902      21.70
 C       4.984456    -1.054116     0.432254     101.29
 H       4.936103    -0.774965     1.424501      27.46
 O       4.501068    -2.458526     0.370032     318.34
 H       4.691936    -2.788461    -0.579224      28.95
 C       6.426280    -1.049427    -0.156891     106.75
 O       6.992381     0.279477    -0.253671     363.61
 H       7.534040     0.539341     0.514064      31.25
 H       6.416575    -1.602913    -1.071325      33.21
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 H       7.146888    -1.704046     0.448587      28.69
55
name= lig-ACN-Water-frame_109
 C      -4.569451     0.259612    -3.397697      53.04
 H      -4.794978    -0.667451    -3.834403      34.24
 C      -3.833232     1.576717    -1.458220      78.69
 H      -3.581661     1.733418    -0.454541      26.92
 C      -3.764140     2.787837    -2.220240      -4.44
 O      -3.353051     3.956443    -1.712163     176.75
 C      -3.122803     4.099514    -0.290365     113.80
 H      -2.329815     3.264582     0.021999      27.95
 H      -3.975808     3.918847     0.273353      28.72
 H      -2.753895     5.043015    -0.116580      27.91
 C      -4.236135     2.717098    -3.589712      -4.46
 O      -4.327531     3.891990    -4.266690      26.40
 H      -4.704734     4.637722    -3.634253      25.07
 C      -4.546783     1.471064    -4.207230      68.46
 H      -4.799384     1.519201    -5.245462      18.06
 C      -4.165795     0.364904    -1.989482       1.85
 C      -4.213696    -0.896793    -1.175488      79.50
 H      -4.825411    -1.610585    -1.763753      23.76
 O      -4.730444    -0.749076     0.142020     207.16
 H      -4.084562    -0.340439     0.848816      22.13
 C      -2.745191    -1.585725    -1.132195      80.56
 H      -2.192414    -1.494919    -2.028457      28.03
 C      -2.843611    -3.097897    -0.790971     122.76
 O      -3.594735    -3.748241    -1.853256     208.84
 H      -2.912018    -4.207557    -2.471318      28.30
 H      -3.378704    -3.323345     0.165639      25.81
 H      -1.778324    -3.510931    -0.636947      25.78
 C       1.722439    -1.381067    -1.153818      46.80
 H       2.379307    -1.840007    -1.886420      19.51
 C       1.631303     0.239193     0.610437      60.33
 H       2.117251     1.004122     1.189150      23.82
 C       0.207786     0.008612     0.688021       6.49
 O      -0.581666     0.592992     1.693798     206.89
 C       0.052738     1.284330     2.818555     107.69
 H      -0.647672     1.191339     3.622542      26.71
 H       1.097717     0.739673     3.103556      24.13
 H       0.230807     2.375000     2.547461      25.16
 C      -0.496498    -0.785632    -0.249386      12.21
 O      -1.896241    -0.866840    -0.097189     138.38
 C       0.289591    -1.502912    -1.196379      73.65
 H      -0.093626    -2.133691    -1.941720      24.83
 C       2.387038    -0.464046    -0.299231      28.75
 C       3.886730    -0.155091    -0.495236      97.42
 H       4.114256    -0.358323    -1.492050      23.94
 O       4.144142     1.259100    -0.232698     263.89
 H       5.201887     1.323079    -0.293252      18.92
 C       4.907506    -1.063716     0.382686      93.42
 H       4.913031    -0.684968     1.354649      27.31
 O       4.464221    -2.442627     0.397980     337.89
 H       4.520658    -2.744222    -0.515628      32.34
 C       6.430647    -1.016221    -0.156297      92.89
 O       7.034641     0.281255    -0.315895     323.00
 H       7.548771     0.376154     0.545273      28.05
 H       6.397009    -1.283006    -1.197972      31.60
 H       6.936617    -1.757819     0.571047      28.13
55
name= lig-ACN-Water-frame_110
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 C      -4.533151     0.280293    -3.389360     167.75
 H      -4.770158    -0.659178    -3.806983      33.92
 C      -3.806787     1.619251    -1.428215      53.86
 H      -3.526529     1.484876    -0.372810      26.94
 C      -3.741652     2.733568    -2.206890       8.43
 O      -3.267778     4.003273    -1.750030     197.38
 C      -3.084381     4.016928    -0.287441     109.58
 H      -2.269030     3.288979     0.140009      28.35
 H      -3.956975     3.932622     0.187104      29.61
 H      -2.721280     5.045336    -0.127409      26.81
 C      -4.168852     2.695842    -3.564286      -1.54
 O      -4.433527     3.849012    -4.272786      -9.65
 H      -4.444258     4.751171    -3.674980      21.85
 C      -4.551683     1.453464    -4.164902      65.40
 H      -4.903382     1.446247    -5.139348      25.85
 C      -4.179023     0.340670    -2.068082     -16.32
 C      -4.100608    -0.915984    -1.146072      60.60
 H      -4.747444    -1.672773    -1.535926      24.25
 O      -4.684779    -0.747986     0.147934     201.76
 H      -4.007042    -0.394259     0.782579      25.47
 C      -2.683627    -1.573855    -1.122330      86.14
 H      -2.350196    -1.448689    -2.165279      29.23
 C      -2.797309    -3.109374    -0.747554     124.84
 O      -3.558323    -3.711520    -1.877950     173.61
 H      -2.816418    -4.053071    -2.451258      29.41
 H      -3.400751    -3.189660     0.166613      27.04
 H      -1.858102    -3.667403    -0.711729      27.02
 C       1.714226    -1.385413    -1.168064      41.43
 H       2.223212    -1.924422    -1.952002      24.44
 C       1.602739     0.270290     0.657871      48.38
 H       1.975065     1.239604     1.124294      21.86
 C       0.228453     0.053611     0.737036      -2.79
 O      -0.596922     0.642056     1.715125     212.17
 C       0.067368     1.312033     2.820753     109.73
 H      -0.623713     1.305560     3.645330      26.96
 H       1.108354     0.800346     3.233078      24.12
 H       0.249357     2.400989     2.571740      24.83
 C      -0.513991    -0.822893    -0.224920       1.68
 O      -1.911152    -0.839184    -0.136811     148.54
 C       0.269963    -1.516127    -1.181755      51.87
 H      -0.257995    -2.041466    -1.997666      23.49
 C       2.389809    -0.527324    -0.259505      34.23
 C       3.816690    -0.158467    -0.554105     111.87
 H       3.959326    -0.297242    -1.594140      23.31
 O       4.140890     1.246904    -0.269813     256.92
 H       5.161737     1.300602    -0.430204      20.53
 C       4.823584    -1.021605     0.288118      97.05
 H       4.744597    -0.656828     1.289421      26.00
 O       4.448688    -2.422810     0.405990     315.98
 H       4.318868    -2.763539    -0.489950      30.94
 C       6.297803    -1.035712    -0.221624     101.55
 O       7.070935     0.307969    -0.346452     292.96
 H       7.498272     0.572865     0.558701      26.23
 H       6.355822    -1.656070    -1.131565      30.65
 H       7.021955    -1.603677     0.450125      27.69
55
name= lig-ACN-Water-frame_111
 C      -4.474309     0.276385    -3.392880      43.23
 H      -4.939448    -0.569692    -3.911711      18.63
 C      -3.772616     1.511320    -1.421719      65.69
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 H      -3.488244     1.636635    -0.325670      23.75
 C      -3.690587     2.749349    -2.208438      -0.80
 O      -3.220235     3.973275    -1.759701     171.07
 C      -3.037195     4.016940    -0.306128     108.69
 H      -2.272838     3.219143    -0.021449      29.26
 H      -3.899695     3.748916     0.152759      27.92
 H      -2.682294     5.072289     0.006794      25.73
 C      -4.185867     2.708583    -3.551053      35.87
 O      -4.500310     3.806907    -4.324706     -13.13
 H      -4.520215     4.685681    -3.707751      20.99
 C      -4.516879     1.493609    -4.128444      32.27
 H      -4.867581     1.500117    -5.120888      30.50
 C      -4.152238     0.323663    -1.972408       0.10
 C      -4.039539    -0.967446    -1.192204      66.74
 H      -4.581343    -1.664145    -1.733287      28.18
 O      -4.684933    -0.757984     0.152824     176.25
 H      -4.156250    -0.374749     0.839098      27.21
 C      -2.634384    -1.601963    -1.104794      96.12
 H      -2.082469    -1.550095    -2.096796      28.14
 C      -2.794703    -3.078319    -0.769839     133.12
 O      -3.484684    -3.710914    -1.898497     206.19
 H      -2.820637    -4.082198    -2.470537      31.53
 H      -3.391889    -3.242182     0.122255      28.46
 H      -1.850732    -3.450912    -0.534455      29.63
 C       1.643567    -1.384378    -1.172099      50.74
 H       2.190718    -1.898081    -1.949301      21.91
 C       1.546665     0.257455     0.634562      54.56
 H       2.189384     0.899529     1.390906      22.43
 C       0.132910     0.036014     0.764929      21.37
 O      -0.611093     0.670882     1.722888     232.59
 C       0.067173     1.381475     2.858189      94.94
 H      -0.664901     1.428462     3.682657      25.93
 H       1.001715     0.639842     3.105198      24.22
 H       0.446902     2.375024     2.528778      26.19
 C      -0.450650    -0.811758    -0.157651      28.49
 O      -1.856498    -0.794555    -0.172702     151.19
 C       0.281160    -1.476182    -1.136146      66.06
 H      -0.172775    -2.204134    -1.907528      23.07
 C       2.293875    -0.469615    -0.292846      24.61
 C       3.829268    -0.206340    -0.624979     100.95
 H       4.013257    -0.416798    -1.685812      24.06
 O       4.139975     1.257769    -0.310436     270.53
 H       5.044695     1.366308    -0.505318      25.47
 C       4.790081    -0.991984     0.227284      97.09
 H       4.759277    -0.540943     1.231009      26.02
 O       4.416755    -2.411495     0.376876     269.60
 H       4.355762    -2.750849    -0.599535      29.07
 C       6.287047    -0.999254    -0.248835      90.03
 O       6.986563     0.278942    -0.408753     295.45
 H       7.653538     0.245851     0.401878      26.51
 H       6.338443    -1.395335    -1.301079      29.47
 H       6.645206    -1.665457     0.572667      27.39
55
name= lig-ACN-Water-frame_112
 C      -4.450521     0.286774    -3.338357      93.50
 H      -4.742943    -0.723284    -3.759614      31.72
 C      -3.685364     1.571002    -1.442313      64.39
 H      -3.399182     1.551028    -0.341120      28.08
 C      -3.663891     2.718588    -2.201105       8.01
 O      -3.203830     3.928731    -1.735898     224.45
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 C      -2.976941     3.980804    -0.332844     113.27
 H      -2.103486     3.392709    -0.009636      30.76
 H      -3.837493     3.818176     0.291944      27.94
 H      -2.695081     5.127297    -0.158985      26.15
 C      -4.234863     2.744518    -3.536012       5.43
 O      -4.527603     3.813793    -4.357843      63.26
 H      -4.716015     4.682452    -3.851880      24.88
 C      -4.471529     1.468897    -4.111394      46.85
 H      -4.813170     1.491286    -5.152782      18.46
 C      -4.086945     0.287720    -2.021490      14.28
 C      -4.071058    -0.987704    -1.183802      81.49
 H      -4.653692    -1.711190    -1.611671      27.83
 O      -4.711835    -0.829649     0.076017     193.04
 H      -4.037245    -0.552134     0.680743      29.45
 C      -2.581194    -1.565628    -1.111578      81.21
 H      -2.127982    -1.531934    -2.191172      27.72
 C      -2.768868    -3.094910    -0.747027     128.15
 O      -3.382509    -3.750893    -1.919443     178.94
 H      -2.589791    -4.127401    -2.411484      28.99
 H      -3.455774    -3.209665     0.069832      27.57
 H      -1.891203    -3.602398    -0.607377      28.66
 C       1.669868    -1.338143    -1.198313      45.10
 H       2.282394    -1.902030    -1.909002      19.40
 C       1.543904     0.198241     0.651638      58.74
 H       2.059818     0.807406     1.518133      21.01
 C       0.185347     0.067172     0.814198      -2.70
 O      -0.688388     0.717788     1.772580     234.63
 C       0.089193     1.371638     2.833901     112.12
 H      -0.732477     1.680273     3.560229      24.83
 H       0.883082     0.736214     3.457570      26.02
 H       0.535027     2.314052     2.472804      26.55
 C      -0.501436    -0.786661    -0.167433      12.14
 O      -1.845579    -0.764861    -0.153062     157.86
 C       0.247050    -1.521113    -1.099635      83.00
 H      -0.331876    -2.286276    -1.765633      22.87
 C       2.307736    -0.372459    -0.437251      44.61
 C       3.761073    -0.144769    -0.640955      93.32
 H       3.953453    -0.366819    -1.731253      23.14
 O       4.118966     1.239950    -0.388387     269.25
 H       5.087950     1.276540    -0.525159      23.27
 C       4.803803    -1.008908     0.230670      82.69
 H       4.747406    -0.621346     1.296089      25.77
 O       4.383380    -2.383432     0.300141     321.25
 H       4.480494    -2.762494    -0.641836      29.21
 C       6.268134    -1.018559    -0.292216     102.05
 O       6.892072     0.254024    -0.418855     328.68
 H       7.610896     0.465764     0.227154      30.19
 H       6.214335    -1.584219    -1.296130      29.83
 H       6.988116    -1.643155     0.231070      27.64
55
name= lig-ACN-Water-frame_113
 C      -4.428070     0.277961    -3.362898      52.05
 H      -4.596513    -0.700241    -3.942246      34.46
 C      -3.603867     1.539989    -1.460304      70.46
 H      -3.167701     1.560649    -0.453950      28.62
 C      -3.699647     2.725981    -2.242260       6.10
 O      -3.204077     3.912620    -1.725155     196.74
 C      -2.863561     4.030282    -0.296553     110.53
 H      -2.032270     3.449279     0.015982      29.21
 H      -3.815935     3.706058     0.258297      26.06
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 H      -2.699790     5.192889    -0.191741      25.73
 C      -4.259550     2.699123    -3.551523      21.58
 O      -4.535478     3.857956    -4.346967      62.90
 H      -4.531291     4.594923    -3.726652      27.13
 C      -4.473021     1.435567    -4.123458      27.27
 H      -4.797276     1.337097    -5.208586      10.82
 C      -4.011202     0.338687    -2.004580      -3.20
 C      -4.044152    -0.999858    -1.244425      80.78
 H      -4.555335    -1.639602    -1.884168      25.69
 O      -4.718513    -0.883231     0.047629     145.40
 H      -4.164372    -0.591756     0.881648      22.58
 C      -2.645287    -1.583501    -1.107139      83.60
 H      -2.138047    -1.341359    -2.157738      28.11
 C      -2.711881    -3.127398    -0.749452     128.20
 O      -3.276922    -3.804114    -1.936009     193.93
 H      -2.469129    -4.172551    -2.460894      28.01
 H      -3.373920    -3.217592     0.105154      26.55
 H      -1.792353    -3.523048    -0.392853      28.27
 C       1.617351    -1.298200    -1.282489      79.92
 H       2.087208    -1.921757    -2.066356      21.18
 C       1.613750     0.207135     0.706381      52.97
 H       2.222161     0.963737     1.290230      19.61
 C       0.135535     0.068473     0.800347       9.32
 O      -0.646682     0.685000     1.769041     208.23
 C       0.048167     1.419465     2.851886      92.80
 H      -0.690595     1.955631     3.545044      24.51
 H       0.651441     0.592399     3.363123      26.12
 H       0.763064     2.102285     2.389577      26.28
 C      -0.474476    -0.733069    -0.178325      14.48
 O      -1.947679    -0.759438    -0.113394     143.77
 C       0.283337    -1.569617    -1.058176      63.28
 H      -0.200829    -2.304238    -1.772613      21.75
 C       2.279215    -0.315334    -0.435199      27.66
 C       3.822451    -0.103149    -0.651052      77.58
 H       4.040715    -0.409389    -1.739944      22.83
 O       4.118504     1.272310    -0.460206     227.23
 H       5.183437     1.346187    -0.469305      19.31
 C       4.781072    -1.047850     0.239578      80.39
 H       4.761360    -0.686292     1.348412      24.50
 O       4.343370    -2.407634     0.202034     358.89
 H       4.433198    -2.679962    -0.715764      28.18
 C       6.262298    -1.109904    -0.348677      92.76
 O       6.809529     0.326688    -0.460716     292.30
 H       7.205966     0.394440     0.400528      31.14
 H       6.231552    -1.429003    -1.449541      30.39
 H       6.784765    -1.749156     0.322718      29.53
55
name= lig-ACN-Water-frame_114
 C      -4.361182     0.255054    -3.391352      35.53
 H      -4.687341    -0.751321    -3.783169      14.55
 C      -3.533700     1.537868    -1.492710      69.97
 H      -3.060128     1.603369    -0.548489      24.00
 C      -3.704936     2.728827    -2.212425     -16.29
 O      -3.195190     3.962503    -1.742579     198.16
 C      -2.813029     4.068054    -0.322347     115.14
 H      -1.931508     3.556392    -0.146124      27.59
 H      -3.642116     3.708841     0.494968      24.09
 H      -2.618343     5.149046    -0.087012      26.51
 C      -4.257477     2.713555    -3.598201      14.01
 O      -4.509308     3.842027    -4.258323      28.24
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 H      -4.601650     4.681133    -3.807085      22.95
 C      -4.524619     1.445242    -4.193859      13.25
 H      -4.843978     1.440507    -5.306522      28.04
 C      -3.997207     0.303307    -2.043572      37.65
 C      -4.007881    -0.976402    -1.265061      98.62
 H      -4.615339    -1.699699    -1.757614      29.56
 O      -4.745317    -0.903210     0.017331     159.88
 H      -3.983617    -0.715562     0.732478      25.49
 C      -2.644925    -1.627454    -1.092657      85.13
 H      -2.000129    -1.669470    -2.090849      26.45
 C      -2.693640    -3.096745    -0.769740     131.79
 O      -3.166173    -3.874305    -1.923594     191.89
 H      -2.368525    -4.093881    -2.451740      30.39
 H      -3.379691    -3.420806     0.025245      26.94
 H      -1.630217    -3.430710    -0.596177      25.59
 C       1.625442    -1.204100    -1.278513      41.34
 H       2.223600    -1.593734    -2.123698      21.61
 C       1.584416     0.265722     0.649881      69.69
 H       2.072762     0.882412     1.356622      22.72
 C       0.226964     0.087888     0.779397      13.25
 O      -0.615224     0.653804     1.749759     214.96
 C       0.086372     1.397048     2.829319     118.11
 H      -0.692651     1.973793     3.303782      25.06
 H       0.490278     0.746440     3.612389      27.38
 H       0.854448     2.098714     2.489796      27.64
 C      -0.575367    -0.763531    -0.162088      12.71
 O      -1.937115    -0.785657    -0.079395     170.61
 C       0.218451    -1.520643    -1.052610      82.34
 H      -0.222437    -2.270725    -1.671985      22.98
 C       2.317316    -0.393618    -0.412529      37.95
 C       3.837277    -0.154569    -0.656042      79.72
 H       4.060926    -0.399485    -1.778882      21.65
 O       4.178128     1.323888    -0.471629     224.61
 H       5.195683     1.413380    -0.565608      19.97
 C       4.768141    -1.085924     0.137543      93.26
 H       4.810173    -0.785718     1.276991      24.36
 O       4.278653    -2.476032     0.105057     343.50
 H       4.234722    -2.771543    -0.827994      28.81
 C       6.187698    -1.038078    -0.373127     109.35
 O       6.731386     0.318945    -0.452030     307.69
 H       7.325632     0.616781     0.319446      28.13
 H       6.256069    -1.508177    -1.403697      31.36
 H       6.876503    -1.622107     0.176841      29.68
55
name= lig-ACN-Water-frame_115
 C      -4.371080     0.285643    -3.472920      50.72
 H      -4.761276    -0.629417    -3.877245      18.53
 C      -3.505646     1.545237    -1.524194      65.91
 H      -3.154570     1.409757    -0.532747      26.38
 C      -3.649582     2.742716    -2.219517       4.46
 O      -3.230182     4.016563    -1.755357     196.56
 C      -2.748955     4.080348    -0.391471     112.36
 H      -1.849380     3.586911    -0.222894      30.65
 H      -3.646859     3.630731     0.342780      25.10
 H      -2.704794     5.130280    -0.268113      28.31
 C      -4.222796     2.687074    -3.503051       1.97
 O      -4.494949     3.866145    -4.249535       5.65
 H      -4.523747     4.600170    -3.644516      24.22
 C      -4.524439     1.465234    -4.173646      22.05
 H      -4.975596     1.481069    -5.221164      28.81
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 C      -3.960755     0.312772    -2.118393     -36.88
 C      -4.030051    -1.034708    -1.251031      78.10
 H      -4.531865    -1.753445    -1.946809      29.92
 O      -4.707667    -0.865738    -0.006884     178.81
 H      -4.163892    -0.636395     0.789427      26.26
 C      -2.596701    -1.621809    -1.082276      81.35
 H      -2.141220    -1.358632    -2.134392      29.63
 C      -2.663108    -3.175328    -0.750751     120.88
 O      -3.087457    -3.937042    -1.923282     222.62
 H      -2.261327    -4.083209    -2.398365      30.80
 H      -3.276129    -3.277205     0.196054      26.54
 H      -1.591787    -3.487446    -0.387316      25.90
 C       1.578873    -1.175065    -1.253238      56.93
 H       1.947332    -1.663164    -2.171075      23.84
 C       1.600711     0.294487     0.589039      58.99
 H       2.067366     0.787316     1.336014      24.54
 C       0.158321     0.064063     0.729261      20.40
 O      -0.540004     0.654113     1.759443     226.62
 C       0.143646     1.353604     2.825633     118.28
 H      -0.480449     1.975577     3.376229      27.00
 H       0.589057     0.654614     3.468594      28.60
 H       0.924772     1.976319     2.373666      27.78
 C      -0.502545    -0.791898    -0.117630      24.49
 O      -1.912091    -0.862382    -0.055989     173.16
 C       0.217131    -1.421289    -1.145080      51.62
 H      -0.223453    -2.061007    -1.808580      22.89
 C       2.373631    -0.361416    -0.363053      30.30
 C       3.805704    -0.121267    -0.689511     103.02
 H       3.877895    -0.310403    -1.858956      21.36
 O       4.239177     1.255300    -0.432818     285.52
 H       5.145327     1.222313    -0.631364      22.84
 C       4.722624    -1.158537     0.083265      88.14
 H       4.567669    -0.846265     1.206981      24.59
 O       4.225467    -2.519394     0.012888     338.60
 H       4.391250    -2.795027    -0.975967      27.75
 C       6.215357    -1.012662    -0.404837      97.18
 O       6.695174     0.356226    -0.454364     322.45
 H       7.407302     0.304520     0.302269      26.87
 H       6.210097    -1.365019    -1.451217      32.20
 H       6.806727    -1.635949     0.240290      28.25
55
name= lig-ACN-Water-frame_116
 C      -4.426445     0.270665    -3.476814      70.08
 H      -4.727331    -0.555438    -4.030283      27.97
 C      -3.512910     1.478366    -1.521569      60.81
 H      -3.152202     1.577531    -0.495428      24.14
 C      -3.559432     2.751674    -2.222472      -4.08
 O      -3.279371     4.012469    -1.798227     198.96
 C      -2.734191     4.115818    -0.459742     117.11
 H      -1.789592     3.611074    -0.396818      30.34
 H      -3.479126     3.573498     0.381501      24.87
 H      -2.614238     5.071474    -0.147501      28.57
 C      -4.212597     2.758224    -3.534489      18.62
 O      -4.468770     3.847683    -4.231541      98.26
 H      -4.469472     4.743006    -3.824494      20.12
 C      -4.512588     1.554159    -4.125714      51.63
 H      -4.945389     1.633471    -5.137358      21.30
 C      -3.928307     0.258060    -2.136994      30.88
 C      -3.959960    -0.984977    -1.300470      69.16
 H      -4.617903    -1.804439    -1.750087      23.25
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 O      -4.714216    -0.824751    -0.012188     182.41
 H      -4.068461    -0.579231     0.611161      28.35
 C      -2.583002    -1.652230    -1.092466      85.41
 H      -1.976974    -1.576429    -2.052170      25.26
 C      -2.588794    -3.170878    -0.731467     114.47
 O      -3.048297    -3.986805    -1.871426     204.98
 H      -2.239672    -4.243419    -2.418591      28.66
 H      -3.477460    -3.418066    -0.065135      24.06
 H      -1.612632    -3.624178    -0.325165      25.80
 C       1.646375    -1.198760    -1.305327      29.06
 H       2.286598    -1.674362    -2.049562      14.87
 C       1.580077     0.295220     0.649531      67.65
 H       2.109647     1.012027     1.179535      21.16
 C       0.223534     0.088992     0.778618       2.40
 O      -0.556929     0.665011     1.781046     216.26
 C       0.300443     1.300705     2.824546     115.68
 H      -0.443605     1.758742     3.440191      25.68
 H       0.804924     0.580883     3.316598      28.47
 H       0.997935     2.056312     2.444536      24.39
 C      -0.507402    -0.806271    -0.162965       9.76
 O      -1.882047    -0.942913    -0.009859     161.34
 C       0.212646    -1.341013    -1.235873      82.80
 H      -0.195903    -1.827881    -2.068425      22.64
 C       2.260166    -0.322881    -0.461400      31.57
 C       3.795481    -0.130963    -0.740841      75.08
 H       3.992289    -0.336220    -1.903155      20.57
 O       4.264266     1.178143    -0.373879     259.47
 H       5.244074     1.151205    -0.349906      17.44
 C       4.667787    -1.157941     0.026409      76.32
 H       4.685331    -0.840140     1.153110      23.08
 O       4.222987    -2.531546    -0.079152     382.92
 H       4.319592    -2.858943    -1.098814      26.27
 C       6.182893    -1.093272    -0.441639      98.97
 O       6.740028     0.382006    -0.425451     300.66
 H       7.352155     0.585867     0.323865      31.10
 H       6.336034    -1.426431    -1.457511      31.76
 H       6.860823    -1.686631     0.184406      29.30
55
name= lig-ACN-Water-frame_117
 C      -4.443521     0.339257    -3.442306     105.74
 H      -4.792180    -0.578155    -3.829017      29.75
 C      -3.499426     1.503734    -1.554797      56.81
 H      -3.137060     1.361310    -0.499479      22.06
 C      -3.579360     2.682605    -2.267115      23.15
 O      -3.296193     4.018465    -1.788264     229.56
 C      -2.704337     4.111194    -0.478363     111.45
 H      -1.686801     3.679929    -0.501137      29.08
 H      -3.367015     3.573368     0.392950      24.99
 H      -2.718244     5.140734    -0.363958      27.40
 C      -4.137268     2.751740    -3.511215       8.96
 O      -4.455056     3.932272    -4.284502     109.30
 H      -4.539499     4.657971    -3.567691      22.37
 C      -4.549073     1.536010    -4.132128      60.87
 H      -4.892368     1.579557    -5.134090      28.77
 C      -3.921085     0.274898    -2.140124       7.82
 C      -3.930124    -1.024060    -1.287529      67.01
 H      -4.503204    -1.754213    -2.019790      23.45
 O      -4.686205    -0.780857    -0.059005     198.31
 H      -4.183330    -0.595982     0.797724      22.18
 C      -2.531071    -1.725146    -1.078976      86.99
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 H      -2.029184    -1.604099    -2.043676      25.51
 C      -2.669720    -3.194277    -0.719613     120.82
 O      -3.035004    -4.041133    -1.822489     219.37
 H      -2.160345    -4.104801    -2.386232      27.59
 H      -3.282726    -3.275509     0.249841      24.45
 H      -1.616505    -3.379803    -0.346947      25.24
 C       1.643825    -1.198536    -1.405740      48.89
 H       2.155813    -1.703027    -2.222422      17.12
 C       1.617546     0.297269     0.594322      44.94
 H       2.114154     1.071033     1.225704      20.59
 C       0.187284     0.029652     0.794462       6.60
 O      -0.531394     0.683902     1.814972     202.69
 C       0.373667     1.249198     2.853984     114.86
 H      -0.241450     1.577308     3.721688      25.67
 H       1.074657     0.592267     3.165662      28.31
 H       0.827326     2.137808     2.429678      25.52
 C      -0.460132    -0.734802    -0.209176      11.60
 O      -1.832737    -0.998447     0.018134     158.41
 C       0.258690    -1.321691    -1.333064      80.60
 H      -0.336625    -1.954423    -2.028775      19.64
 C       2.310410    -0.261403    -0.520056      30.58
 C       3.772242    -0.158671    -0.745101      89.19
 H       3.948625    -0.235979    -1.925432      22.74
 O       4.237519     1.174492    -0.309147     232.00
 H       5.257076     1.066089    -0.177435      18.37
 C       4.709448    -1.179146    -0.033399      80.38
 H       4.573391    -0.976990     1.087501      24.25
 O       4.235243    -2.530692    -0.128368     344.37
 H       4.196901    -2.756758    -1.175851      25.46
 C       6.193311    -1.062649    -0.455858      96.51
 O       6.761202     0.317280    -0.414131     316.24
 H       7.360196     0.239091     0.330736      29.52
 H       6.245456    -1.422435    -1.458856      31.54
 H       6.763224    -1.751289     0.232418      27.93
55
name= lig-ACN-Water-frame_118
 C      -4.458583     0.315569    -3.395088      70.00
 H      -4.955905    -0.528432    -3.886698      19.94
 C      -3.439769     1.510866    -1.534285      59.21
 H      -3.013227     1.623437    -0.487149      19.90
 C      -3.614682     2.763329    -2.251348       9.21
 O      -3.304936     3.950430    -1.769530     183.89
 C      -2.668385     4.132795    -0.485949     120.44
 H      -1.585079     3.775910    -0.408023      27.33
 H      -3.264724     3.583677     0.342741      24.61
 H      -2.690112     5.191113    -0.180535      25.48
 C      -4.167525     2.756648    -3.669593      13.65
 O      -4.404486     3.948210    -4.264024      70.16
 H      -4.478031     4.853616    -3.738268      23.52
 C      -4.576786     1.522071    -4.201065      45.47
 H      -5.043188     1.473534    -5.134088      24.92
 C      -3.902273     0.304290    -2.100923      34.52
 C      -3.905139    -1.004938    -1.297514      76.71
 H      -4.548546    -1.864437    -1.806574      25.48
 O      -4.687317    -0.792998    -0.113914     187.92
 H      -3.994920    -0.529410     0.651553      22.90
 C      -2.581007    -1.682536    -1.064074      93.84
 H      -2.048722    -1.625251    -1.973440      27.28
 C      -2.635496    -3.216890    -0.626023     116.58
 O      -3.058578    -4.085158    -1.757924     167.27
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 H      -2.276137    -4.148408    -2.363819      29.53
 H      -3.457663    -3.479840     0.121963      25.01
 H      -1.693707    -3.635007    -0.291081      25.54
 C       1.632468    -1.085528    -1.497454      32.53
 H       2.112743    -1.569485    -2.338841      23.20
 C       1.592041     0.281349     0.463072      62.12
 H       2.260448     0.841496     1.250348      20.74
 C       0.258995     0.060133     0.742762      16.76
 O      -0.454778     0.633282     1.844034     215.38
 C       0.400863     1.235955     2.870238     115.12
 H      -0.177008     1.211427     3.842389      25.42
 H       1.251941     0.628686     2.975045      26.95
 H       0.721552     2.229793     2.605346      27.23
 C      -0.444596    -0.726202    -0.251444      22.55
 O      -1.772316    -1.047096    -0.018781     179.59
 C       0.241305    -1.312713    -1.292494      65.33
 H      -0.146453    -2.136617    -2.026774      19.79
 C       2.328406    -0.343434    -0.564404      31.33
 C       3.843432    -0.083825    -0.752437      97.94
 H       4.055681    -0.172940    -1.926778      21.75
 O       4.187194     1.207761    -0.236418     222.53
 H       5.241691     1.307706    -0.394320      18.59
 C       4.691333    -1.188287    -0.021724      92.31
 H       4.658714    -0.903074     1.064302      26.20
 O       4.253921    -2.547285    -0.178944     304.34
 H       4.350986    -2.841988    -1.181381      27.91
 C       6.197574    -1.088244    -0.488344     104.29
 O       6.780575     0.207095    -0.407137     301.10
 H       7.399150     0.300513     0.336255      27.13
 H       6.293052    -1.375861    -1.524886      32.24
 H       6.820920    -1.802919     0.143826      28.89
55
name= lig-ACN-Water-frame_119
 C      -4.488237     0.334869    -3.411475      51.92
 H      -4.874244    -0.687428    -3.702455      29.54
 C      -3.409739     1.577088    -1.572084      61.87
 H      -2.930173     1.627588    -0.577114      23.40
 C      -3.656320     2.688360    -2.321174      11.84
 O      -3.285652     4.006019    -1.757673     214.35
 C      -2.660178     4.120598    -0.432978     102.74
 H      -1.554737     3.775664    -0.596809      27.40
 H      -3.138830     3.557134     0.358377      26.31
 H      -2.754223     5.273938    -0.281179      24.82
 C      -4.199804     2.742180    -3.605352       7.59
 O      -4.358467     3.971343    -4.321012      83.45
 H      -4.302253     4.654452    -3.560607      24.34
 C      -4.586437     1.508140    -4.205669      59.20
 H      -5.067376     1.488058    -5.153545      22.04
 C      -3.876746     0.321242    -2.114536       5.79
 C      -3.935500    -0.970054    -1.307372      58.22
 H      -4.490878    -1.690064    -2.086007      24.75
 O      -4.720400    -0.837397    -0.104092     197.98
 H      -4.268403    -0.426021     0.753823      21.19
 C      -2.525998    -1.752315    -1.042703      89.05
 H      -2.058112    -1.746183    -1.962897      27.93
 C      -2.648883    -3.258212    -0.593705     122.23
 O      -3.085446    -4.104765    -1.695084     183.53
 H      -2.355391    -4.218588    -2.300426      31.33
 H      -3.429872    -3.282078     0.203360      25.38
 H      -1.723241    -3.454860    -0.120060      27.26
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 C       1.624981    -1.046455    -1.604247      25.30
 H       2.154537    -1.461519    -2.457894      25.87
 C       1.681892     0.262620     0.445411      46.06
 H       2.274629     0.975815     1.193756      20.00
 C       0.260859     0.127356     0.651004      18.54
 O      -0.354505     0.537357     1.809410     203.76
 C       0.451048     1.193818     2.874530     108.24
 H      -0.198157     1.040576     3.781753      25.47
 H       1.464592     0.776200     3.096317      25.18
 H       0.489191     2.255393     2.736428      26.42
 C      -0.451940    -0.756080    -0.225430      16.40
 O      -1.794411    -1.027163    -0.015457     176.10
 C       0.283332    -1.340675    -1.306587      61.54
 H      -0.380621    -1.984427    -2.004199      18.00
 C       2.385451    -0.333810    -0.631136      32.87
 C       3.860340    -0.084587    -0.749951      80.83
 H       4.229002    -0.021106    -1.874528      19.56
 O       4.159038     1.290766    -0.182144     228.58
 H       5.068267     1.460968    -0.485789      20.59
 C       4.745327    -1.169192    -0.031465      91.53
 H       4.655082    -1.005205     1.030860      24.81
 O       4.263751    -2.560024    -0.217819     354.34
 H       4.315763    -2.797801    -1.184451      28.20
 C       6.197200    -1.208001    -0.511042      94.68
 O       6.802318     0.175985    -0.458411     342.99
 H       7.285475     0.370551     0.388846      27.78
 H       6.145309    -1.523097    -1.556950      32.09
 H       6.803610    -1.996510     0.034232      28.41
55
name= lig-ACN-Water-frame_120
 C      -4.471446     0.347217    -3.390313      55.12
 H      -4.945197    -0.553687    -3.924129      21.16
 C      -3.407040     1.543820    -1.617858      65.80
 H      -2.925667     1.476017    -0.671359      25.87
 C      -3.589747     2.820752    -2.267774       2.26
 O      -3.308305     4.031833    -1.803268     167.24
 C      -2.660319     4.094631    -0.467480     110.46
 H      -1.506618     3.784411    -0.399309      27.33
 H      -3.159362     3.568904     0.228033      29.05
 H      -2.722537     5.243558    -0.089860      25.16
 C      -4.237573     2.759429    -3.591137       3.12
 O      -4.311484     3.924800    -4.322084      74.73
 H      -4.349934     4.753000    -3.839091      23.62
 C      -4.615039     1.509537    -4.158326      57.96
 H      -4.924318     1.516262    -5.222699      23.36
 C      -3.869051     0.331782    -2.149446      32.49
 C      -3.880124    -1.000911    -1.295888      60.20
 H      -4.567955    -1.757995    -1.892153      23.53
 O      -4.813698    -0.900523    -0.111002     144.97
 H      -4.208108    -0.720774     0.666809      25.82
 C      -2.561397    -1.770083    -1.064410      90.88
 H      -2.003602    -1.741578    -1.943896      28.73
 C      -2.695283    -3.213290    -0.544382     128.22
 O      -3.063376    -4.116102    -1.634025     155.74
 H      -2.215032    -4.162089    -2.193071      29.22
 H      -3.358707    -3.357286     0.285434      27.64
 H      -1.768511    -3.631134    -0.258412      27.99
 C       1.662620    -1.077022    -1.619383      39.67
 H       1.975710    -1.488125    -2.580563      18.47
 C       1.731082     0.261281     0.437488      50.71
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 H       2.292017     0.997229     1.108456      22.95
 C       0.364324     0.094612     0.600115       4.81
 O      -0.266590     0.462927     1.794780     195.82
 C       0.434210     1.161796     2.876245     105.90
 H      -0.079701     0.966577     3.822148      25.95
 H       1.536161     0.756041     2.932503      24.84
 H       0.472935     2.210389     2.599344      25.98
 C      -0.380501    -0.790592    -0.256643       5.66
 O      -1.823225    -0.970873     0.005504     119.83
 C       0.286324    -1.329849    -1.365828      70.75
 H      -0.141830    -1.928392    -2.176730      23.44
 C       2.393254    -0.239132    -0.699530      27.82
 C       3.919218    -0.038417    -0.748604      83.94
 H       4.151470    -0.062839    -1.897842      24.03
 O       4.140960     1.332692    -0.174195     233.62
 H       5.067773     1.459625    -0.240994      23.11
 C       4.770977    -1.231817    -0.042676      88.31
 H       4.737625    -1.012102     0.988150      26.47
 O       4.243355    -2.540218    -0.247241     361.15
 H       4.314238    -2.785437    -1.163266      30.17
 C       6.233002    -1.202565    -0.537951     106.58
 O       6.801555     0.103047    -0.570564     329.17
 H       7.359270     0.184290     0.290706      27.37
 H       6.279149    -1.548025    -1.590526      30.34
 H       6.836680    -1.858468     0.152437      27.69
55
name= lig-ACN-Water-frame_121
 C      -4.491266     0.312421    -3.448530      25.27
 H      -4.857258    -0.651068    -3.897092      24.78
 C      -3.369936     1.563640    -1.587887      53.50
 H      -2.897736     1.630382    -0.653437      21.60
 C      -3.598337     2.772352    -2.275853      18.38
 O      -3.263417     4.111060    -1.787946     214.80
 C      -2.702795     4.094058    -0.497232     114.51
 H      -1.601085     3.624827    -0.615957      25.43
 H      -3.224569     3.507504     0.110818      28.40
 H      -2.716599     5.237355    -0.119311      24.17
 C      -4.199169     2.794674    -3.530059      22.87
 O      -4.298272     3.904755    -4.363924     123.27
 H      -4.388873     4.690466    -3.796068      23.31
 C      -4.607792     1.603515    -4.097400      55.38
 H      -5.055724     1.554680    -5.145775      23.43
 C      -3.883197     0.255358    -2.127947      -2.81
 C      -3.957698    -1.047700    -1.325615      81.24
 H      -4.357754    -1.853238    -2.080778      26.14
 O      -4.824581    -0.948364    -0.148329     181.85
 H      -4.370617    -0.650005     0.625284      26.74
 C      -2.583607    -1.668302    -0.982026      89.39
 H      -2.126196    -1.746323    -1.957383      28.11
 C      -2.656509    -3.207920    -0.493271     114.09
 O      -2.978507    -4.110240    -1.606044     162.06
 H      -2.208050    -4.184846    -2.267566      29.28
 H      -3.450805    -3.336561     0.174808      26.56
 H      -1.707634    -3.279963    -0.007080      27.20
 C       1.717008    -1.067668    -1.570846      41.81
 H       2.355854    -1.479785    -2.359950      20.51
 C       1.770118     0.313776     0.367311      53.30
 H       2.336515     0.815689     1.109323      23.63
 C       0.412339    -0.049376     0.684936       6.67
 O      -0.264594     0.385885     1.792253     210.50
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 C       0.463361     1.139380     2.802468     111.83
 H      -0.091027     0.953150     3.694446      26.74
 H       1.567214     0.704290     3.039621      23.02
 H       0.494319     2.244731     2.668225      25.94
 C      -0.399575    -0.797719    -0.308025      12.72
 O      -1.725451    -0.924602    -0.044234     171.39
 C       0.304717    -1.304468    -1.447184      52.29
 H      -0.208127    -1.908797    -2.091868      22.93
 C       2.439770    -0.231416    -0.752722      30.10
 C       3.922968    -0.003523    -0.800825     101.62
 H       4.430106     0.088492    -1.824463      23.14
 O       4.184042     1.315741    -0.200529     215.55
 H       5.227009     1.311405    -0.175292      16.89
 C       4.763095    -1.201020    -0.073893      89.25
 H       4.756169    -1.090831     0.960323      26.13
 O       4.189886    -2.530548    -0.275486     324.62
 H       4.426465    -2.903447    -1.175569      28.63
 C       6.276311    -1.237748    -0.555749     102.76
 O       6.841833     0.097578    -0.667758     285.37
 H       7.360170     0.443828     0.245024      24.30
 H       6.342229    -1.798276    -1.544147      30.17
 H       6.868181    -1.866840     0.124739      27.94
55
name= lig-ACN-Water-frame_122
 C      -4.461058     0.369208    -3.401766      69.06
 H      -4.931894    -0.462749    -3.889707      20.54
 C      -3.401221     1.496528    -1.563789      62.18
 H      -2.946953     1.385184    -0.588336      21.46
 C      -3.579487     2.795772    -2.238993       7.52
 O      -3.255649     4.080493    -1.835179     213.96
 C      -2.703178     4.090840    -0.467412     112.48
 H      -1.584139     3.674990    -0.402062      26.22
 H      -3.281089     3.626945     0.254210      27.52
 H      -2.617608     5.196730    -0.134463      25.41
 C      -4.154497     2.793060    -3.562196       5.17
 O      -4.310923     3.947240    -4.368747     107.97
 H      -4.219189     4.812373    -3.811022      24.31
 C      -4.630178     1.537355    -4.089530      40.37
 H      -5.187770     1.751882    -5.063497      23.25
 C      -3.911733     0.327569    -2.134492      34.74
 C      -3.961733    -1.036495    -1.321013      79.93
 H      -4.484814    -1.825152    -1.957210      25.58
 O      -4.847760    -0.958260    -0.212031     191.08
 H      -4.323562    -0.579601     0.496325      28.51
 C      -2.540275    -1.682717    -0.968395      92.04
 H      -2.035999    -1.631951    -1.964341      26.49
 C      -2.610013    -3.115428    -0.466143     128.23
 O      -2.829354    -4.082329    -1.565665     193.07
 H      -2.050708    -3.993638    -2.124210      30.42
 H      -3.360524    -3.264813     0.258236      26.74
 H      -1.744442    -3.565042     0.035706      25.78
 C       1.760875    -1.098005    -1.629463      25.05
 H       2.159752    -1.756594    -2.418911      22.82
 C       1.737153     0.307596     0.396702      53.64
 H       2.209897     0.943496     1.016599      26.14
 C       0.437203    -0.147667     0.666445      22.02
 O      -0.280614     0.310057     1.802226     192.93
 C       0.471963     1.106967     2.789042     100.90
 H      -0.085805     1.127643     3.698039      26.54
 H       1.589768     0.675466     2.991953      22.97
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 H       0.576543     2.132432     2.302284      26.29
 C      -0.276968    -0.762131    -0.352876      21.76
 O      -1.688900    -0.870773    -0.103994     179.65
 C       0.370955    -1.280608    -1.466697      67.24
 H      -0.087159    -1.811759    -2.226402      21.69
 C       2.470378    -0.227651    -0.702800       4.45
 C       3.983920    -0.024256    -0.868915     110.73
 H       4.136322    -0.020486    -1.984458      21.63
 O       4.305755     1.276054    -0.217035     213.86
 H       5.327544     1.435703    -0.458105      16.48
 C       4.780318    -1.181445    -0.136821      91.37
 H       4.619256    -0.895570     0.854791      26.11
 O       4.146672    -2.504378    -0.303887     291.11
 H       4.329041    -2.836083    -1.287043      26.78
 C       6.272018    -1.272261    -0.524579      94.98
 O       6.890593     0.131597    -0.731300     278.91
 H       7.347923     0.318547     0.218410      25.78
 H       6.309691    -1.648490    -1.610876      28.69
 H       6.846065    -1.809134     0.212341      27.80
55
name= lig-ACN-Water-frame_123
 C      -4.516273     0.369273    -3.400723      29.75
 H      -4.945977    -0.523135    -3.735225      25.80
 C      -3.453150     1.566248    -1.535365      59.61
 H      -2.989429     1.600510    -0.503157      20.44
 C      -3.565538     2.736357    -2.274915      18.16
 O      -3.207350     3.994820    -1.790005     203.13
 C      -2.685781     4.145686    -0.422319     114.41
 H      -1.685500     3.548864    -0.325192      26.22
 H      -3.432050     3.669036     0.241143      26.37
 H      -2.638723     5.218456    -0.280088      25.72
 C      -4.134679     2.786530    -3.610042      34.88
 O      -4.315744     3.961323    -4.309373     160.20
 H      -4.232294     4.787004    -3.692394      22.51
 C      -4.638772     1.628523    -4.145287      63.53
 H      -5.085929     1.376293    -5.127544      22.11
 C      -3.906101     0.316256    -2.092715      20.65
 C      -3.863533    -0.995132    -1.351542      79.29
 H      -4.281064    -1.722857    -2.070924      27.86
 O      -4.869971    -0.913848    -0.217833     138.24
 H      -4.435293    -0.708023     0.703711      23.15
 C      -2.459878    -1.657464    -1.078461      80.45
 H      -1.960725    -1.858209    -2.098408      28.41
 C      -2.538773    -3.117633    -0.418406     112.42
 O      -2.724322    -4.030631    -1.515017     187.57
 H      -1.931963    -4.023632    -2.080717      30.49
 H      -3.401033    -3.194985     0.229183      26.21
 H      -1.541879    -3.097105     0.088909      25.99
 C       1.833440    -1.093396    -1.626610       2.08
 H       2.435132    -1.428582    -2.491737      14.12
 C       1.796490     0.254144     0.426206      59.72
 H       2.216964     1.013493     0.982158      23.20
 C       0.418580    -0.066251     0.683429       6.10
 O      -0.274650     0.202959     1.823102     195.38
 C       0.460754     1.096533     2.719365     110.36
 H      -0.156985     1.272938     3.607374      25.41
 H       1.447749     0.546797     3.097439      22.73
 H       0.741777     2.127377     2.277302      24.06
 C      -0.303778    -0.795780    -0.367700      22.09
 O      -1.665360    -0.797508    -0.149733     147.96
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 C       0.440230    -1.278790    -1.508809      48.01
 H      -0.130531    -1.770255    -2.322875      22.16
 C       2.467008    -0.298862    -0.715388      40.05
 C       3.976100    -0.041628    -0.907250     106.87
 H       4.279675     0.019162    -1.961921      23.60
 O       4.453344     1.223379    -0.299835     283.89
 H       5.319328     1.373324    -0.637325      22.40
 C       4.751314    -1.172165    -0.191623      90.24
 H       4.726621    -1.011484     0.868541      26.09
 O       4.150807    -2.455081    -0.342482     339.64
 H       4.035411    -2.692927    -1.331670      28.40
 C       6.282845    -1.165120    -0.552124     106.72
 O       6.901725     0.100988    -0.703613     323.40
 H       7.420648     0.356231     0.047540      31.05
 H       6.425608    -1.836871    -1.495819      30.70
 H       6.815755    -1.763166     0.164995      29.09
55
name= lig-ACN-Water-frame_124
 C      -4.550698     0.401688    -3.362305      60.58
 H      -4.903678    -0.456975    -3.840049      23.32
 C      -3.496800     1.581834    -1.526810      56.04
 H      -3.098866     1.707319    -0.441306      20.52
 C      -3.560406     2.737976    -2.314293      13.85
 O      -3.133870     3.952591    -1.759128     233.18
 C      -2.729336     4.139216    -0.416224     121.88
 H      -1.715465     3.670418    -0.167824      27.55
 H      -3.437881     3.900206     0.485250      25.95
 H      -2.556733     5.143025    -0.314274      27.48
 C      -4.149229     2.779934    -3.599785       4.31
 O      -4.305048     3.998515    -4.246141     173.99
 H      -4.345874     4.753637    -3.622614      23.80
 C      -4.621221     1.530991    -4.177240      55.15
 H      -4.972011     1.764989    -5.155370      22.59
 C      -3.898026     0.374084    -2.112228      40.22
 C      -3.821867    -0.979377    -1.379304      83.16
 H      -4.284938    -1.719994    -1.982352      25.37
 O      -4.817596    -0.907942    -0.227631     170.63
 H      -4.212044    -0.538179     0.591600      21.86
 C      -2.449654    -1.607031    -1.072673      98.01
 H      -1.935849    -1.573813    -2.138678      23.73
 C      -2.436597    -2.995158    -0.446755     119.88
 O      -2.675098    -4.042863    -1.430763     193.35
 H      -1.870619    -4.062802    -2.067671      27.82
 H      -3.237825    -3.162935     0.338314      24.68
 H      -1.548213    -3.346096     0.168693      25.84
 C       1.835190    -1.066477    -1.648820      77.69
 H       2.308274    -1.325651    -2.610727      11.55
 C       1.835588     0.215720     0.433989      59.68
 H       2.491886     0.701344     1.177789      20.66
 C       0.444401    -0.056101     0.597656      12.73
 O      -0.248199     0.159037     1.841394     199.78
 C       0.430579     1.081168     2.714310     107.51
 H      -0.360091     1.341350     3.486937      24.25
 H       1.333170     0.616858     3.255675      23.76
 H       0.744152     2.008181     2.101565      24.22
 C      -0.243583    -0.785054    -0.372290      23.53
 O      -1.666260    -0.761033    -0.262942     165.69
 C       0.433032    -1.280983    -1.510341      89.27
 H      -0.089671    -1.840088    -2.392267      20.41
 C       2.536713    -0.242640    -0.681207      20.93
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 C       3.998448    -0.040118    -0.902667     102.66
 H       4.130628    -0.164485    -1.974637      25.24
 O       4.526692     1.205871    -0.415635     266.92
 H       5.455377     1.044124    -0.561635      19.83
 C       4.776967    -1.154603    -0.195190      86.97
 H       4.619150    -0.897702     0.872597      24.58
 O       4.173547    -2.457379    -0.397607     336.07
 H       4.192469    -2.664059    -1.359459      29.90
 C       6.291130    -1.205925    -0.567776      97.46
 O       6.947838     0.143135    -0.675929     324.36
 H       7.181406     0.378281     0.187801      32.92
 H       6.423095    -1.629649    -1.625175      29.31
 H       6.770749    -1.730286     0.248613      28.18
55
name= lig-ACN-Water-frame_125
 C      -4.524146     0.374991    -3.415693      40.41
 H      -4.921155    -0.569614    -3.773369      26.88
 C      -3.505417     1.565140    -1.540402      67.73
 H      -3.087872     1.426443    -0.472933      23.86
 C      -3.556072     2.779938    -2.220245      13.03
 O      -3.090609     3.980780    -1.808111     197.33
 C      -2.714647     4.156249    -0.350984     104.31
 H      -1.862878     3.532547    -0.088691      28.50
 H      -3.709421     3.780475     0.230803      25.03
 H      -2.567620     5.148891    -0.305467      27.45
 C      -4.165102     2.796750    -3.551375      22.90
 O      -4.303704     3.991338    -4.227803     135.06
 H      -4.224728     4.795007    -3.704393      22.19
 C      -4.575456     1.614439    -4.164179      65.60
 H      -5.099426     1.411800    -5.022224      24.57
 C      -3.931647     0.355238    -2.137201      32.17
 C      -3.913889    -0.973038    -1.371061      90.35
 H      -4.322087    -1.673719    -2.018192      28.59
 O      -4.696463    -0.925283    -0.240978     204.37
 H      -4.262883    -0.584483     0.673117      20.16
 C      -2.427116    -1.546323    -1.124469      77.30
 H      -2.008983    -1.715465    -2.222393      25.88
 C      -2.382947    -2.971270    -0.456871     106.08
 O      -2.679988    -4.091097    -1.343664     173.45
 H      -1.947623    -4.031531    -2.080953      28.17
 H      -3.185407    -2.882880     0.362058      24.26
 H      -1.301497    -2.957865    -0.086766      24.73
 C       1.797853    -0.945595    -1.659008      46.72
 H       2.291113    -1.446583    -2.489580      25.69
 C       1.870699     0.183766     0.478417      52.41
 H       2.352046     0.567722     1.466908      21.23
 C       0.510011    -0.097313     0.635830       6.74
 O      -0.193581     0.132667     1.768874     220.63
 C       0.373505     1.102170     2.746093     105.53
 H      -0.410960     1.441331     3.540817      25.10
 H       1.207835     0.670785     3.308122      24.37
 H       0.749987     2.036069     2.206920      25.89
 C      -0.252633    -0.727813    -0.447568      16.38
 O      -1.611037    -0.656522    -0.293889     157.08
 C       0.463513    -1.274994    -1.498648      85.88
 H      -0.084029    -1.882295    -2.321680      20.72
 C       2.514402    -0.221897    -0.739340      35.99
 C       4.041238    -0.073380    -0.962369     108.77
 H       4.248593    -0.159583    -2.010201      23.74
 O       4.570631     1.226362    -0.544018     255.58
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 H       5.581836     1.196794    -0.582074      15.14
 C       4.811377    -1.190196    -0.182042      90.83
 H       4.747732    -1.028443     0.947594      25.01
 O       4.237178    -2.479857    -0.426006     341.62
 H       4.337095    -2.810243    -1.338345      28.43
 C       6.314226    -1.222535    -0.547551      97.34
 O       6.977919     0.178521    -0.609823     306.85
 H       7.418897     0.490720     0.240732      26.62
 H       6.343615    -1.594193    -1.604843      31.13
 H       6.956939    -1.969150    -0.041591      29.07
55
name= lig-ACN-Water-frame_126
 C      -4.443297     0.386031    -3.481802      54.05
 H      -4.969123    -0.451725    -4.029508      22.29
 C      -3.480201     1.510587    -1.521188      50.68
 H      -2.948187     1.542044    -0.542300      20.25
 C      -3.596636     2.768798    -2.202711       1.65
 O      -3.009869     4.074797    -1.791284     228.91
 C      -2.770692     4.137877    -0.385695     117.41
 H      -1.981550     3.531047    -0.071552      27.99
 H      -3.743449     3.844540     0.315973      24.25
 H      -2.502620     5.097343    -0.033729      27.37
 C      -4.159070     2.831230    -3.486232      13.40
 O      -4.303700     3.963443    -4.266377     128.83
 H      -4.236692     4.791263    -3.696011      22.82
 C      -4.596512     1.610994    -4.108208      56.34
 H      -4.926505     1.874381    -5.054213      21.37
 C      -3.985465     0.318563    -2.149652      29.73
 C      -3.861559    -0.987329    -1.430890      99.70
 H      -4.312851    -1.727314    -1.976568      27.87
 O      -4.683918    -0.965838    -0.154913     158.95
 H      -4.029140    -0.793173     0.600524      23.67
 C      -2.468384    -1.538192    -1.240588      75.08
 H      -1.883131    -1.497783    -2.252016      24.10
 C      -2.337580    -2.901765    -0.468442     108.36
 O      -2.705256    -4.106669    -1.246342     176.83
 H      -2.059532    -4.202437    -1.976901      30.47
 H      -2.946437    -3.122166     0.510773      23.88
 H      -1.302983    -3.102150    -0.061354      24.35
 C       1.820433    -0.894216    -1.716385      45.90
 H       2.429688    -1.222341    -2.550808      22.12
 C       1.930474     0.119290     0.485904      56.23
 H       2.621191     0.754094     1.217727      20.28
 C       0.551862    -0.149866     0.633331      18.62
 O      -0.197417     0.174067     1.780094     209.83
 C       0.342839     1.121186     2.760161     101.78
 H      -0.624441     1.222375     3.407539      24.06
 H       1.080048     0.669911     3.348383      25.69
 H       0.675745     2.096311     2.336144      25.60
 C      -0.229015    -0.620823    -0.445619      11.18
 O      -1.621557    -0.560358    -0.326802     120.29
 C       0.434981    -1.238721    -1.537953      80.24
 H      -0.061486    -1.850881    -2.298819      20.33
 C       2.574773    -0.152060    -0.735420      23.98
 C       4.090621    -0.097257    -0.992972      81.51
 H       4.298694    -0.336994    -2.005123      23.88
 O       4.567251     1.270619    -0.652662     216.01
 H       5.599904     1.125892    -0.889115      15.41
 C       4.877621    -1.234787    -0.165959      73.47
 H       4.668464    -1.021750     0.962337      22.92
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 O       4.322764    -2.546031    -0.383985     363.43
 H       4.271365    -2.666830    -1.376793      26.22
 C       6.402662    -1.146872    -0.599856      99.58
 O       6.994371     0.129889    -0.564028     348.44
 H       7.296607     0.339105     0.416903      24.96
 H       6.437696    -1.423120    -1.646589      31.45
 H       6.944808    -1.819556     0.123955      27.45
55
name= lig-ACN-Water-frame_127
 C      -4.448965     0.404577    -3.514597       5.60
 H      -4.672713    -0.583552    -4.080330      25.84
 C      -3.473075     1.551088    -1.549011      64.22
 H      -3.053709     1.364423    -0.590143      26.52
 C      -3.544714     2.835842    -2.173570     -16.06
 O      -2.997007     4.044124    -1.774248     180.48
 C      -2.796292     4.118827    -0.330557     113.52
 H      -2.075607     3.472851    -0.044022      29.21
 H      -3.842880     3.860699     0.223629      24.31
 H      -2.492438     5.190388    -0.244768      26.02
 C      -4.176636     2.840889    -3.472114      34.69
 O      -4.291222     3.942320    -4.290943      32.28
 H      -4.401180     4.842983    -3.772733      18.56
 C      -4.595449     1.692090    -4.112870      59.43
 H      -4.937921     1.668935    -5.128979      24.58
 C      -3.955841     0.350129    -2.165129     -27.21
 C      -3.887618    -1.058610    -1.407324      91.23
 H      -4.361460    -1.744527    -1.999010      29.43
 O      -4.648589    -1.023242    -0.131205     149.76
 H      -4.103690    -0.645361     0.586055      27.37
 C      -2.376164    -1.517089    -1.196164      83.15
 H      -2.004524    -1.636990    -2.281465      30.14
 C      -2.278911    -2.908517    -0.479388     116.84
 O      -2.743476    -4.096477    -1.179887     186.01
 H      -2.029180    -4.220085    -1.807873      32.80
 H      -2.961043    -2.602966     0.404431      26.18
 H      -1.203383    -2.980239    -0.249440      26.93
 C       1.857677    -0.866251    -1.743547      29.80
 H       2.138063    -1.103703    -2.753714      17.57
 C       1.988991     0.121967     0.457864      48.29
 H       2.481290     0.655982     1.377280      19.95
 C       0.581244    -0.075563     0.664360      -9.54
 O      -0.207278     0.224727     1.770418     217.50
 C       0.286222     1.112125     2.809299     122.21
 H      -0.522667     1.394459     3.572568      23.93
 H       1.103238     0.742207     3.313460      24.74
 H       0.558199     2.037501     2.314316      26.22
 C      -0.221993    -0.625190    -0.470572      -9.06
 O      -1.678983    -0.530512    -0.403569     147.75
 C       0.491527    -1.090019    -1.593151      69.74
 H       0.009696    -1.574777    -2.360066      26.12
 C       2.618394    -0.215069    -0.788142      52.95
 C       4.098908    -0.111798    -0.974306     104.34
 H       4.236564    -0.272112    -2.005537      25.49
 O       4.591432     1.245069    -0.747690     267.19
 H       5.604527     1.311932    -0.757859      15.81
 C       4.930181    -1.190558    -0.201493      77.41
 H       4.949417    -0.935277     0.948865      22.57
 O       4.428430    -2.586883    -0.310767     317.79
 H       4.350705    -2.910825    -1.285044      26.76
 C       6.429607    -1.195450    -0.599501     105.24
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 O       7.025348     0.147533    -0.583378     386.25
 H       7.398820     0.522807     0.290565      27.78
 H       6.532737    -1.585843    -1.575554      32.39
 H       7.035504    -1.928312     0.006570      29.26
55
name= lig-ACN-Water-frame_128
 C      -4.440339     0.439106    -3.461214      64.15
 H      -4.706797    -0.520037    -4.050550      23.82
 C      -3.494619     1.575582    -1.552579      68.99
 H      -3.114040     1.623518    -0.586695      28.98
 C      -3.536054     2.787421    -2.248831       8.95
 O      -3.003720     3.984829    -1.726115     218.08
 C      -2.797518     4.133929    -0.294809     120.78
 H      -2.117781     3.534382     0.146658      29.15
 H      -3.814876     4.033234     0.252171      26.31
 H      -2.448451     5.234225    -0.029361      25.92
 C      -4.185198     2.871441    -3.511157      11.37
 O      -4.284866     3.995921    -4.311057      73.31
 H      -4.211785     4.917591    -3.773817      18.27
 C      -4.579634     1.629983    -4.146493      51.70
 H      -5.074531     1.739409    -5.153310      20.00
 C      -3.908666     0.347902    -2.166204      18.03
 C      -3.868513    -1.010555    -1.378489      90.11
 H      -4.303705    -1.776341    -1.946219      26.35
 O      -4.603440    -1.060941    -0.158604     165.90
 H      -4.112025    -0.716636     0.599072      26.53
 C      -2.378080    -1.548261    -1.228701      90.40
 H      -1.901172    -1.610226    -2.234459      28.09
 C      -2.224654    -2.855021    -0.432667     115.36
 O      -2.756441    -4.034061    -1.141536     162.49
 H      -2.148625    -4.332988    -1.904734      28.69
 H      -2.760999    -3.030801     0.553178      26.34
 H      -1.218425    -3.074267    -0.105412      27.53
 C       1.875814    -0.824264    -1.803288      32.38
 H       2.529667    -1.111369    -2.635134      21.50
 C       1.942113     0.149811     0.456217      54.50
 H       2.635926     0.395211     1.291562      21.08
 C       0.513157     0.004364     0.596305       5.48
 O      -0.231069     0.248893     1.751417     206.16
 C       0.306339     1.166093     2.836722     114.71
 H      -0.545606     1.195810     3.513661      25.66
 H       1.103216     0.682193     3.316350      26.49
 H       0.572636     2.126088     2.483686      27.85
 C      -0.213961    -0.591189    -0.445347      13.54
 O      -1.610759    -0.546351    -0.472544     163.83
 C       0.456421    -0.931570    -1.646133      61.30
 H      -0.090981    -1.200180    -2.459946      26.49
 C       2.630476    -0.299778    -0.719435       6.89
 C       4.171544    -0.148662    -1.061546      94.21
 H       4.354598    -0.431441    -2.080658      23.12
 O       4.600315     1.215771    -0.767621     279.75
 H       5.528855     1.020958    -0.635889      15.05
 C       5.010291    -1.201387    -0.201879      89.41
 H       4.849016    -0.876187     0.909889      20.64
 O       4.535836    -2.565828    -0.217884     290.72
 H       4.443671    -2.722011    -1.236905      27.62
 C       6.481207    -1.248289    -0.611062      99.39
 O       7.070830     0.177766    -0.686914     340.11
 H       7.369228     0.402125     0.253572      28.77
 H       6.523411    -1.558271    -1.603401      32.05
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 H       7.008229    -1.874309     0.132965      28.68
55
name= lig-ACN-Water-frame_129
 C      -4.426701     0.392990    -3.435191      34.00
 H      -5.005138    -0.487673    -3.841037      21.36
 C      -3.505069     1.564879    -1.527905      77.80
 H      -3.083490     1.577632    -0.548542      25.18
 C      -3.571175     2.766392    -2.288648      -1.55
 O      -2.997731     3.968469    -1.693422     189.56
 C      -2.829002     4.147103    -0.244480     109.39
 H      -2.123398     3.472291     0.104684      27.90
 H      -3.756149     4.084490     0.353064      26.43
 H      -2.345615     5.248504    -0.286875      24.46
 C      -4.143286     2.871407    -3.624353      18.00
 O      -4.278251     4.049707    -4.327493      38.06
 H      -4.236577     4.904223    -3.702082      20.01
 C      -4.576785     1.645498    -4.148430      56.85
 H      -5.052032     1.659060    -5.201296      20.28
 C      -3.886176     0.351518    -2.095885      -0.39
 C      -3.750941    -0.990073    -1.423723      77.90
 H      -4.304368    -1.613060    -2.109795      26.20
 O      -4.577838    -1.054994    -0.154128     109.14
 H      -3.959973    -0.857686     0.654185      25.78
 C      -2.367667    -1.561889    -1.210077      82.09
 H      -2.046777    -1.810107    -2.221831      29.66
 C      -2.196832    -2.911128    -0.366087     119.69
 O      -2.761849    -3.977772    -1.141480     173.18
 H      -2.101044    -4.001736    -1.911144      29.66
 H      -2.714925    -2.681918     0.555135      27.65
 H      -1.141969    -2.985632    -0.309597      28.55
 C       1.857072    -0.771369    -1.778952      64.47
 H       2.212993    -1.164768    -2.742502      20.80
 C       1.920430     0.126544     0.458742      57.92
 H       2.375263     0.568890     1.296129      22.78
 C       0.516940     0.052575     0.590883      -3.56
 O      -0.234443     0.323566     1.738313     214.91
 C       0.320857     1.137616     2.823532     127.56
 H      -0.467075     1.253632     3.472204      26.35
 H       1.169984     0.680584     3.335917      25.37
 H       0.558165     2.098005     2.462531      26.87
 C      -0.184296    -0.501668    -0.576514       3.14
 O      -1.569651    -0.546067    -0.467634     149.49
 C       0.471082    -0.807147    -1.755650      68.77
 H      -0.098337    -1.115680    -2.601920      27.69
 C       2.645128    -0.334575    -0.717441      40.82
 C       4.176385    -0.252156    -1.029623     104.43
 H       4.223931    -0.399234    -2.106233      22.50
 O       4.604193     1.132437    -0.756382     306.02
 H       5.523484     1.274168    -0.810165      21.76
 C       5.066634    -1.170929    -0.161298      87.91
 H       5.031407    -0.754669     0.915200      23.61
 O       4.611856    -2.540550    -0.177874     288.78
 H       4.311132    -2.796488    -1.081517      30.02
 C       6.574694    -1.158608    -0.629616     112.76
 O       7.111588     0.139239    -0.774175     325.77
 H       7.332335     0.580739     0.161499      26.58
 H       6.641318    -1.698810    -1.532518      31.57
 H       7.222504    -1.709136     0.036667      29.55
55
name= lig-ACN-Water-frame_130
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 C      -4.468477     0.418690    -3.407848      84.38
 H      -4.879493    -0.505992    -3.798157      25.88
 C      -3.483131     1.600353    -1.532593      72.42
 H      -3.030643     1.571636    -0.513321      24.25
 C      -3.565522     2.829199    -2.205789       4.04
 O      -3.048711     3.966499    -1.731639     202.61
 C      -2.824802     4.134777    -0.270355     114.55
 H      -2.147610     3.427457     0.231918      26.38
 H      -3.740144     4.117645     0.223425      27.18
 H      -2.385683     5.229290    -0.085070      24.84
 C      -4.056000     2.854600    -3.596916      16.85
 O      -4.267212     4.051663    -4.345419      87.03
 H      -4.258800     4.903468    -3.785186      23.42
 C      -4.564888     1.598668    -4.147563      55.81
 H      -5.059152     1.491295    -5.164233      21.93
 C      -3.887074     0.364022    -2.132327      19.18
 C      -3.776276    -1.018964    -1.387371      83.38
 H      -4.175903    -1.881604    -1.992726      27.62
 O      -4.522019    -1.038319    -0.163415     144.58
 H      -3.919777    -0.727107     0.666866      23.76
 C      -2.262006    -1.565125    -1.166048      95.19
 H      -1.758933    -1.674330    -2.086492      29.98
 C      -2.189610    -2.841883    -0.371373     129.79
 O      -2.752068    -3.948649    -1.153667     179.65
 H      -2.231961    -4.119941    -1.929236      31.44
 H      -2.646386    -2.965658     0.559443      28.99
 H      -1.195075    -3.095962    -0.106049      29.32
 C       1.874368    -0.755130    -1.824971      55.07
 H       2.509299    -0.971940    -2.696945      15.23
 C       1.973889     0.127658     0.478862      68.91
 H       2.504281     0.597759     1.197515      24.30
 C       0.535037     0.028534     0.530720      -0.25
 O      -0.239663     0.375680     1.660344     198.67
 C       0.351677     1.131647     2.786615     117.09
 H      -0.374849     1.334650     3.471956      27.29
 H       1.172809     0.520997     3.252058      25.10
 H       0.765384     2.056076     2.427489      27.10
 C      -0.228675    -0.351628    -0.627111       6.79
 O      -1.585405    -0.537475    -0.448757     178.74
 C       0.451507    -0.723436    -1.824858      60.98
 H      -0.036545    -1.176202    -2.746128      27.02
 C       2.629764    -0.320441    -0.711200      22.51
 C       4.148847    -0.275520    -0.914338     100.45
 H       4.387030    -0.645157    -1.944745      24.33
 O       4.549167     1.102172    -0.734191     265.06
 H       5.459378     1.002047    -1.239463      20.43
 C       5.154585    -1.167107    -0.142874      90.20
 H       5.127344    -0.888649     0.934221      26.13
 O       4.660438    -2.547284    -0.132349     297.21
 H       4.455011    -2.709669    -1.059876      30.90
 C       6.630628    -1.147803    -0.626000     103.78
 O       7.203669     0.211745    -0.846592     205.18
 H       7.441658     0.533406     0.182876      23.82
 H       6.672419    -1.565143    -1.619278      32.13
 H       7.133737    -1.706436     0.111818      30.63
55
name= lig-ACN-Water-frame_131
 C      -4.498197     0.396765    -3.400461      47.64
 H      -4.749559    -0.441538    -3.970401      25.93
 C      -3.454433     1.565238    -1.531657      56.83
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 H      -3.015249     1.596671    -0.471245      22.38
 C      -3.563936     2.799073    -2.238927       9.80
 O      -3.056934     4.083191    -1.721312     214.84
 C      -2.862294     4.128524    -0.315655     116.74
 H      -2.119447     3.298513     0.015279      25.86
 H      -3.728327     4.050817     0.189555      29.05
 H      -2.381822     5.157639    -0.168385      25.54
 C      -4.081674     2.821577    -3.539725      21.44
 O      -4.230226     3.982979    -4.329709     137.76
 H      -4.052508     4.715961    -3.735927      25.33
 C      -4.517736     1.642817    -4.113522      58.95
 H      -4.946986     1.851447    -5.097444      21.85
 C      -3.881304     0.333818    -2.109826       6.79
 C      -3.730343    -1.040954    -1.375785      80.60
 H      -4.372420    -1.776701    -2.016093      22.19
 O      -4.466396    -1.016123    -0.112658     168.16
 H      -3.901243    -0.566729     0.589799      26.85
 C      -2.261727    -1.482088    -1.165665      87.95
 H      -1.891370    -1.659145    -2.116392      27.76
 C      -2.166477    -2.891534    -0.353967     113.57
 O      -2.754650    -3.950883    -1.186543     209.46
 H      -2.018997    -4.111390    -1.831380      29.63
 H      -2.799555    -2.680453     0.410183      27.48
 H      -1.151099    -3.047700    -0.091078      27.49
 C       1.900868    -0.686950    -1.857181      53.66
 H       2.368561    -1.000759    -2.781164      24.30
 C       1.967496     0.135868     0.466310      62.91
 H       2.544008     0.323106     1.303809      20.67
 C       0.561939     0.092809     0.503042       8.24
 O      -0.248144     0.415397     1.561326     197.41
 C       0.441691     1.114328     2.706326     106.15
 H      -0.408310     1.317578     3.298053      26.48
 H       1.086768     0.367130     3.275263      24.50
 H       0.974660     2.042016     2.424889      26.97
 C      -0.204224    -0.312355    -0.667855      10.94
 O      -1.582093    -0.448672    -0.378185     186.95
 C       0.483208    -0.680014    -1.826344      58.46
 H      -0.186472    -1.004133    -2.742304      20.59
 C       2.630414    -0.344121    -0.699500      30.32
 C       4.154996    -0.295050    -0.856146      82.59
 H       4.220624    -0.526926    -1.965414      20.07
 O       4.516958     1.125366    -0.752733     271.51
 H       5.488833     1.400856    -1.018646      18.37
 C       5.152277    -1.202895    -0.028868      91.51
 H       5.246920    -0.858306     0.978264      24.67
 O       4.720422    -2.563359    -0.113845     310.41
 H       4.705195    -2.862087    -1.075252      28.06
 C       6.649890    -1.124077    -0.667165     101.33
 O       7.286406     0.266127    -0.826303     218.23
 H       7.407509     0.726239     0.151609      24.37
 H       6.641500    -1.613570    -1.675870      31.03
 H       7.335219    -1.669172    -0.084621      29.50
55
name= lig-ACN-Water-frame_132
 C      -4.437418     0.392655    -3.433221      68.88
 H      -4.873914    -0.464176    -3.826426      28.01
 C      -3.437290     1.553210    -1.532566      53.83
 H      -2.994589     1.460500    -0.484114      22.58
 C      -3.489521     2.824194    -2.191749       4.05
 O      -3.119092     4.095134    -1.790580     190.18
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 C      -2.859016     4.146611    -0.323832     115.43
 H      -2.066100     3.308526     0.000842      25.33
 H      -3.694511     4.040669     0.246507      29.35
 H      -2.391938     5.089093    -0.073180      27.15
 C      -4.124605     2.828203    -3.482178      25.14
 O      -4.161005     3.937883    -4.270943     102.91
 H      -4.108568     4.802326    -3.820337      19.36
 C      -4.534747     1.632802    -4.095559      63.43
 H      -4.872243     1.525257    -5.091711      24.21
 C      -3.895297     0.322633    -2.117202       3.56
 C      -3.736095    -0.960647    -1.342754      79.84
 H      -4.169129    -1.897904    -1.980271      25.24
 O      -4.416504    -0.972766    -0.024033     156.12
 H      -3.836033    -0.627159     0.640312      28.08
 C      -2.286770    -1.480691    -1.170411      84.62
 H      -1.831506    -1.493388    -2.094682      28.57
 C      -2.227406    -2.825285    -0.392078     119.97
 O      -2.704111    -3.948681    -1.209594     199.13
 H      -2.011332    -4.179312    -1.948283      27.34
 H      -2.741924    -2.927384     0.497618      27.38
 H      -1.225433    -3.082133    -0.087095      27.13
 C       1.881937    -0.623921    -1.856790      34.27
 H       2.356271    -0.899195    -2.778515      21.33
 C       1.967175     0.078574     0.452402      64.86
 H       2.405114     0.288615     1.443884      19.42
 C       0.556876     0.185779     0.449818      19.62
 O      -0.200350     0.511375     1.531038     229.21
 C       0.457387     1.049707     2.637878     112.15
 H      -0.233145     1.585997     3.339711      24.11
 H       1.122086     0.307054     3.198671      24.46
 H       1.148432     1.860882     2.240235      25.13
 C      -0.164105    -0.327116    -0.624007      23.73
 O      -1.544691    -0.380738    -0.394635     173.53
 C       0.488819    -0.648776    -1.813836      56.06
 H      -0.022564    -0.955315    -2.834322      21.82
 C       2.677254    -0.355589    -0.715307      40.33
 C       4.205394    -0.264327    -0.886891      74.42
 H       4.567854    -0.640803    -1.923844      18.98
 O       4.490759     1.208024    -0.748020     261.77
 H       5.426557     1.116491    -0.662097      17.74
 C       5.191560    -1.171942    -0.045378      90.31
 H       5.158168    -0.933595     0.958034      25.08
 O       4.793128    -2.604911    -0.079500     308.24
 H       4.748836    -2.827618    -1.089930      26.63
 C       6.670801    -1.028471    -0.677973      99.01
 O       7.270629     0.252228    -0.749366     309.79
 H       7.450994     0.571891     0.230128      28.98
 H       6.495106    -1.284924    -1.778308      30.96
 H       7.268282    -1.781709    -0.169052      28.87
55
name= lig-ACN-Water-frame_133
 C      -4.392707     0.354022    -3.401037      62.77
 H      -4.808280    -0.516828    -3.861210      20.28
 C      -3.406615     1.581295    -1.499970      72.33
 H      -2.966502     1.543641    -0.498569      21.14
 C      -3.523042     2.778144    -2.193867      11.08
 O      -3.156442     4.056722    -1.751211     215.09
 C      -2.812130     4.186368    -0.347600     119.60
 H      -2.002202     3.368143     0.035423      23.42
 H      -3.725909     4.035344     0.185463      26.90
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 H      -2.472791     5.133884    -0.246482      27.00
 C      -4.120013     2.783868    -3.480450       1.36
 O      -4.111693     3.992902    -4.252400      53.82
 H      -4.198771     4.788497    -3.599022      19.98
 C      -4.563316     1.565910    -4.101935      60.32
 H      -4.970316     1.759976    -5.063966      21.12
 C      -3.878355     0.397613    -2.107482      25.75
 C      -3.757081    -0.931509    -1.266986      72.19
 H      -4.440789    -1.785818    -1.815148      22.91
 O      -4.384492    -0.903520     0.041036     187.32
 H      -3.707392    -0.650078     0.737849      23.81
 C      -2.284239    -1.394584    -1.141483      95.68
 H      -1.908848    -1.689587    -2.083732      26.70
 C      -2.225357    -2.814077    -0.426232     108.67
 O      -2.676721    -3.941691    -1.236432     221.96
 H      -2.006187    -3.995253    -1.999148      27.63
 H      -2.887777    -2.735370     0.414215      25.25
 H      -1.159026    -2.852532    -0.164134      25.32
 C       1.936493    -0.606452    -1.868070      48.77
 H       2.455009    -0.659207    -2.810067      16.30
 C       2.015759     0.023031     0.448009      57.04
 H       2.765434     0.382181     1.273088      15.97
 C       0.606678     0.183997     0.444163       8.26
 O      -0.213223     0.598429     1.510316     203.89
 C       0.574735     1.093001     2.662912      83.24
 H      -0.286119     1.587878     3.297404      21.65
 H       0.932267     0.180564     3.225505      22.96
 H       1.420576     1.828072     2.384086      20.90
 C      -0.183047    -0.334525    -0.648851      17.14
 O      -1.555242    -0.408321    -0.471318     212.44
 C       0.490021    -0.640371    -1.819593      54.08
 H      -0.126696    -1.036921    -2.697871      22.05
 C       2.710092    -0.335052    -0.734968      32.33
 C       4.226357    -0.212422    -0.930498      68.23
 H       4.272542    -0.359078    -2.091915      17.29
 O       4.526087     1.204666    -0.709487     291.86
 H       5.427136     1.464168    -0.656071      17.54
 C       5.220679    -1.128499    -0.087488      88.33
 H       5.254468    -0.784199     0.905485      21.12
 O       4.879791    -2.572704    -0.083298     312.57
 H       4.636115    -2.815944    -1.025724      26.94
 C       6.597016    -1.047365    -0.689836     102.75
 O       7.235850     0.281820    -0.637402     359.42
 H       7.291159     0.578574     0.354050      31.68
 H       6.553777    -1.274314    -1.827925      29.17
 H       7.296705    -1.804235    -0.228913      27.24
55
name= lig-ACN-Water-frame_134
 C      -4.408143     0.355451    -3.366000      18.61
 H      -4.593244    -0.658579    -3.803057      26.53
 C      -3.402337     1.609102    -1.449435      61.16
 H      -3.028317     1.659447    -0.471448      21.37
 C      -3.593854     2.781175    -2.209940      -0.16
 O      -3.158341     3.996442    -1.711409     209.89
 C      -2.801563     4.228171    -0.353753     123.95
 H      -1.844733     3.590404    -0.031289      24.59
 H      -3.556255     4.082620     0.449253      25.81
 H      -2.487795     5.169536    -0.320753      27.67
 C      -4.084943     2.802059    -3.573020      26.84
 O      -4.111233     3.990354    -4.208536      46.33
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 H      -3.967979     4.841843    -3.598019      20.22
 C      -4.555686     1.612469    -4.114235      63.06
 H      -5.065871     1.498100    -5.082885      21.00
 C      -3.843351     0.361640    -2.010918     -10.71
 C      -3.783631    -0.879372    -1.215978      84.04
 H      -4.390738    -1.713405    -1.874344      22.74
 O      -4.383919    -0.808465     0.112047     193.45
 H      -3.731719    -0.421028     0.876460      19.91
 C      -2.358412    -1.477515    -1.230987      84.18
 H      -2.085122    -1.378361    -2.268659      28.51
 C      -2.189693    -2.778532    -0.418605     114.07
 O      -2.672246    -3.888899    -1.241830     227.24
 H      -2.037073    -4.071465    -1.937549      28.74
 H      -2.836903    -2.805455     0.510909      24.55
 H      -1.197293    -3.076109    -0.007330      24.81
 C       1.934781    -0.598642    -1.931691      28.48
 H       2.355967    -0.774907    -2.919980      21.23
 C       2.053499     0.040934     0.445865      49.56
 H       2.572495     0.400941     1.465210      15.66
 C       0.620644     0.090915     0.501864       5.88
 O      -0.131622     0.698841     1.482774     193.01
 C       0.608448     1.112460     2.740776      95.23
 H      -0.129991     1.827682     3.394382      22.32
 H       1.014117     0.247628     3.312821      24.46
 H       1.491005     1.811668     2.430647      23.21
 C      -0.112163    -0.322780    -0.667488       5.75
 O      -1.557143    -0.409500    -0.497344     142.62
 C       0.564674    -0.688647    -1.862272      55.93
 H       0.016214    -0.987299    -2.736659      21.15
 C       2.712645    -0.311660    -0.778308      54.94
 C       4.222136    -0.154303    -0.973680      81.57
 H       4.588874    -0.412653    -2.073390      16.54
 O       4.543947     1.226823    -0.633047     276.94
 H       5.536740     1.150189    -1.004183      14.71
 C       5.186191    -1.095735    -0.168742      91.69
 H       5.181185    -0.730674     0.850582      21.12
 O       4.904372    -2.488264    -0.099605     333.70
 H       4.781879    -2.775379    -1.026634      27.24
 C       6.636711    -1.039311    -0.741859      75.76
 O       7.175068     0.301463    -0.609916     374.16
 H       7.231993     0.670456     0.368037      28.89
 H       6.604613    -1.379455    -1.861809      29.74
 H       7.241897    -1.784341    -0.088132      28.22
55
name= lig-ACN-Water-frame_135
 C      -4.373679     0.448244    -3.267914      81.32
 H      -4.814642    -0.486958    -3.769868      16.20
 C      -3.493308     1.601120    -1.445183      89.42
 H      -3.108408     1.663115    -0.485130      25.48
 C      -3.591547     2.775753    -2.167284       6.17
 O      -3.188559     4.008884    -1.726196     200.27
 C      -2.716880     4.262159    -0.312904     112.44
 H      -1.784567     3.642402    -0.070757      26.15
 H      -3.594246     3.980202     0.378187      25.23
 H      -2.488840     5.263240    -0.293305      27.53
 C      -4.054224     2.798944    -3.529272      -4.92
 O      -4.136970     4.009231    -4.245387     100.30
 H      -3.900549     4.776581    -3.608716      18.89
 C      -4.519744     1.540654    -4.088681      43.33
 H      -4.820318     1.494532    -5.186755      24.61
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 C      -3.876120     0.411259    -2.012429      46.26
 C      -3.802509    -0.914652    -1.153803      67.71
 H      -4.546899    -1.764752    -1.576944      24.61
 O      -4.415546    -0.716770     0.150523     167.92
 H      -3.622854    -0.524185     0.897655      21.66
 C      -2.332721    -1.462937    -1.221437      69.97
 H      -1.975791    -1.792718    -2.231577      27.48
 C      -2.177500    -2.800481    -0.445502     109.25
 O      -2.720752    -3.870071    -1.223997     216.54
 H      -2.031379    -4.072871    -1.887798      29.38
 H      -2.814967    -2.689415     0.537070      25.68
 H      -1.063520    -2.807399    -0.246105      25.82
 C       1.993838    -0.613781    -1.970521      40.63
 H       2.594649    -0.925787    -2.846670      20.71
 C       2.044436     0.057112     0.393913      45.84
 H       2.758233     0.253935     1.314530      17.94
 C       0.656522     0.051053     0.497111       6.94
 O      -0.021607     0.771393     1.537222     208.74
 C       0.626121     1.149545     2.743308     100.18
 H      -0.231530     1.770957     3.364615      23.19
 H       0.911838     0.267230     3.356754      25.34
 H       1.541310     1.821708     2.508270      24.67
 C      -0.141237    -0.401176    -0.661711      15.59
 O      -1.477695    -0.396631    -0.526005     162.66
 C       0.529012    -0.726585    -1.861338      62.07
 H       0.004584    -1.002004    -2.694003      24.97
 C       2.717361    -0.270822    -0.821918      38.75
 C       4.213678    -0.160196    -0.998521      78.98
 H       4.292846    -0.215316    -2.180603      17.32
 O       4.584357     1.240409    -0.623396     261.86
 H       5.616818     1.485465    -0.637176      14.87
 C       5.205231    -1.051929    -0.213101      87.85
 H       5.209052    -0.670161     0.851732      20.71
 O       4.824911    -2.453299    -0.137281     320.12
 H       4.816261    -2.750675    -1.096245      27.53
 C       6.655933    -0.975805    -0.702779      93.11
 O       7.135019     0.360266    -0.704534     329.86
 H       7.298877     0.492878     0.330117      29.24
 H       6.771385    -1.241047    -1.819887      29.08
 H       7.318663    -1.713673    -0.081967      28.06
55
name= lig-ACN-Water-frame_136
 C      -4.434982     0.361678    -3.305557      40.30
 H      -4.914640    -0.630216    -3.682518      27.42
 C      -3.543898     1.644343    -1.348074      69.15
 H      -3.179718     1.613281    -0.329429      25.22
 C      -3.566498     2.827902    -2.156123      -3.43
 O      -3.179131     4.117438    -1.688513     188.85
 C      -2.675782     4.230339    -0.365444     120.40
 H      -1.783630     3.642300    -0.147580      28.32
 H      -3.469239     3.979770     0.490068      25.69
 H      -2.419434     5.290310    -0.224416      27.50
 C      -4.079408     2.822344    -3.493773      22.80
 O      -4.156636     3.942618    -4.281996      89.40
 H      -4.079101     4.791538    -3.796432      23.07
 C      -4.395386     1.629884    -4.065060      50.61
 H      -4.768531     1.623508    -5.152479      16.13
 C      -3.955142     0.358627    -1.929956     -31.99
 C      -3.801580    -0.885745    -1.153114      78.33
 H      -4.355715    -1.740515    -1.756806      25.53
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 O      -4.410923    -0.671478     0.182526     169.51
 H      -3.677191    -0.359505     0.921082      22.10
 C      -2.314999    -1.418911    -1.102986      92.15
 H      -2.095297    -1.407953    -2.240315      28.02
 C      -2.155444    -2.767332    -0.436555     108.82
 O      -2.783583    -3.890536    -1.197595     208.60
 H      -2.167764    -4.103294    -2.002948      28.00
 H      -2.560399    -2.851615     0.693125      24.82
 H      -1.080295    -3.138748    -0.309650      25.46
 C       1.935890    -0.678170    -1.941325      45.78
 H       2.334731    -0.843238    -2.966591      21.73
 C       2.091655     0.048308     0.344751      54.80
 H       2.690581     0.460341     1.203928      20.73
 C       0.673111     0.122061     0.468254      15.56
 O       0.003341     0.735965     1.496269     213.95
 C       0.673545     1.181605     2.776142      94.47
 H      -0.195217     1.815131     3.314989      23.53
 H       0.947834     0.293822     3.386742      24.92
 H       1.540608     1.874175     2.648304      23.16
 C      -0.054339    -0.464672    -0.612014      13.03
 O      -1.500521    -0.417012    -0.566534     192.74
 C       0.586704    -0.767860    -1.854437      58.32
 H      -0.031239    -1.136461    -2.584102      24.89
 C       2.738824    -0.262452    -0.861500      33.36
 C       4.263030    -0.071430    -1.025783      81.32
 H       4.587458    -0.259918    -2.158170      22.11
 O       4.563362     1.297125    -0.642436     257.31
 H       5.486264     1.168323    -0.433027      17.63
 C       5.192464    -1.065957    -0.210752      77.64
 H       5.150630    -0.699511     0.890629      21.52
 O       4.714581    -2.422773    -0.180682     321.71
 H       4.528231    -2.801479    -1.131570      26.78
 C       6.650066    -0.939782    -0.724653      94.29
 O       7.165192     0.491430    -0.754416     292.17
 H       7.386348     0.880475     0.222249      27.05
 H       6.639877    -1.424279    -1.753645      29.23
 H       7.349032    -1.497840    -0.032769      27.46
55
name= lig-ACN-Water-frame_137
 C      -4.444664     0.376797    -3.285949      81.87
 H      -4.690600    -0.560240    -3.883191      26.53
 C      -3.601961     1.673206    -1.357769      82.66
 H      -3.245734     1.734027    -0.290297      24.77
 C      -3.566587     2.903679    -2.055467       3.27
 O      -3.188606     4.178432    -1.682880     199.93
 C      -2.618764     4.212384    -0.354821     117.43
 H      -1.799621     3.575795    -0.335021      28.77
 H      -3.419967     3.881975     0.463054      25.12
 H      -2.217500     5.295520    -0.180408      26.28
 C      -4.044109     2.847854    -3.428043      -2.38
 O      -4.183693     3.911167    -4.324022     119.23
 H      -3.952458     4.760847    -3.931282      23.94
 C      -4.364775     1.536717    -4.035099      11.15
 H      -4.746515     1.614627    -5.096693      13.99
 C      -4.029671     0.454066    -1.957667      23.28
 C      -3.794633    -0.853006    -1.076259      84.33
 H      -4.386433    -1.756283    -1.473441      23.50
 O      -4.406767    -0.690037     0.199987     173.35
 H      -3.734839    -0.219045     0.774994      27.65
 C      -2.342721    -1.382508    -1.109326      69.09
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 H      -2.075987    -1.633943    -2.229237      26.89
 C      -2.115297    -2.869287    -0.425646      99.65
 O      -2.863319    -3.881219    -1.160584     201.91
 H      -2.276872    -4.047495    -1.990019      28.34
 H      -2.636813    -2.824975     0.650620      24.72
 H      -0.975228    -2.976118    -0.396184      25.59
 C       1.991572    -0.733149    -1.977378      32.14
 H       2.439351    -0.830261    -2.989494      20.21
 C       2.141147     0.121478     0.341831      59.68
 H       2.686879     0.592636     1.101822      21.91
 C       0.743947     0.149785     0.418686       8.03
 O      -0.018553     0.691182     1.494643     202.47
 C       0.681177     1.176809     2.748435     101.66
 H      -0.083938     1.800430     3.342270      24.71
 H       1.082458     0.337724     3.376238      25.46
 H       1.475125     1.796528     2.377569      24.25
 C      -0.089632    -0.469775    -0.601416      25.52
 O      -1.449520    -0.366917    -0.490232     176.70
 C       0.522497    -0.872852    -1.753134      61.66
 H       0.034372    -1.202237    -2.660780      24.54
 C       2.791287    -0.286327    -0.913892      25.26
 C       4.268131    -0.035251    -1.049631      83.92
 H       4.580587    -0.142503    -2.181050      20.13
 O       4.560089     1.340960    -0.640114     268.95
 H       5.450019     1.577556    -0.770502      21.14
 C       5.123786    -1.020580    -0.193130      66.91
 H       5.046280    -0.678436     0.932583      22.75
 O       4.604666    -2.380018    -0.199767     303.84
 H       4.793875    -2.674974    -1.212388      25.70
 C       6.674195    -0.876634    -0.701051     106.82
 O       7.157335     0.582600    -0.778279     271.91
 H       7.421935     0.708120     0.162592      30.75
 H       6.827075    -1.111617    -1.773334      30.40
 H       7.316866    -1.461783    -0.048738      28.96
55
name= lig-ACN-Water-frame_138
 C      -4.380813     0.397753    -3.242132      23.40
 H      -4.600956    -0.598111    -3.647710      24.97
 C      -3.653390     1.745525    -1.359028      37.27
 H      -3.306821     1.619636    -0.274835      22.94
 C      -3.670393     2.935601    -2.122560       6.90
 O      -3.205694     4.204178    -1.648303     201.64
 C      -2.525388     4.191551    -0.324418     109.97
 H      -1.757223     3.547332    -0.232929      30.17
 H      -3.328018     3.953672     0.496826      24.30
 H      -2.206068     5.362686    -0.134256      24.40
 C      -4.027584     2.794086    -3.473161      27.41
 O      -4.186637     3.897154    -4.320673     151.53
 H      -3.880435     4.722872    -3.848219      20.46
 C      -4.391518     1.611801    -4.024168      80.06
 H      -4.534054     1.538185    -5.094884      29.39
 C      -4.014128     0.467354    -1.890505     -19.00
 C      -3.835737    -0.816155    -1.083491      78.81
 H      -4.444129    -1.555550    -1.647775      25.46
 O      -4.385252    -0.691368     0.276217     182.89
 H      -3.774305    -0.367361     0.909477      27.45
 C      -2.326744    -1.428312    -1.086790      75.54
 H      -1.964161    -1.431604    -2.224407      28.39
 C      -2.167237    -2.827076    -0.433448     112.07
 O      -2.898095    -3.864373    -1.148905     212.90
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 H      -2.381191    -4.141396    -1.902567      31.35
 H      -2.495539    -2.867750     0.695621      25.07
 H      -1.080660    -3.184202    -0.418928      25.70
 C       1.976167    -0.779846    -1.934083      45.11
 H       2.434550    -1.117278    -2.863705      21.40
 C       2.176789     0.215818     0.263441      62.87
 H       2.793117     0.557387     0.973990      22.74
 C       0.735513     0.135869     0.453323      11.05
 O      -0.019371     0.631579     1.528546     213.06
 C       0.702983     1.162327     2.609947     122.59
 H      -0.054808     1.657518     3.222058      26.64
 H       1.127963     0.311230     3.210080      26.12
 H       1.442878     1.893223     2.416833      27.30
 C      -0.057611    -0.411575    -0.609030       0.63
 O      -1.464469    -0.356270    -0.386923     137.00
 C       0.614578    -0.991987    -1.778693      62.67
 H      -0.157158    -1.374050    -2.522609      24.79
 C       2.765710    -0.245146    -0.896649      36.16
 C       4.269967    -0.006022    -1.093229      87.78
 H       4.482400    -0.132528    -2.217948      20.52
 O       4.542816     1.387931    -0.630544     257.12
 H       5.376323     1.623377    -1.188465      20.31
 C       5.144834    -0.924821    -0.237941      71.49
 H       5.022615    -0.497621     0.865504      22.77
 O       4.566437    -2.293589    -0.227027     317.97
 H       4.828040    -2.815119    -1.098944      25.70
 C       6.648760    -0.767034    -0.669319     114.55
 O       7.129941     0.585941    -0.720621     362.92
 H       7.269527     0.986891     0.104549      34.03
 H       6.623282    -1.257863    -1.649608      31.76
 H       7.320046    -1.336807    -0.095522      28.74
55
name= lig-ACN-Water-frame_139
 C      -4.320891     0.418642    -3.209789      80.19
 H      -4.666891    -0.488863    -3.629139      22.97
 C      -3.684480     1.786514    -1.293835      75.42
 H      -3.358817     2.075343    -0.257620      20.46
 C      -3.705638     2.934787    -2.099317       1.36
 O      -3.226525     4.163680    -1.614105     214.68
 C      -2.525041     4.183063    -0.331404     108.42
 H      -1.707608     3.566326    -0.370765      28.63
 H      -3.183683     3.976264     0.534370      25.58
 H      -2.048166     5.341191    -0.309148      24.03
 C      -4.069797     2.868019    -3.526554      -0.93
 O      -4.151265     3.948827    -4.318914     100.67
 H      -3.929267     4.864144    -3.851278      22.26
 C      -4.399110     1.539098    -4.063711      51.18
 H      -4.687515     1.519185    -5.075966      24.60
 C      -3.941901     0.511205    -1.825282      15.82
 C      -3.813553    -0.807052    -1.056096      67.30
 H      -4.375966    -1.591959    -1.506750      25.83
 O      -4.356443    -0.698416     0.326807     198.76
 H      -3.635213    -0.404210     0.865971      26.82
 C      -2.337969    -1.342533    -1.037085      84.07
 H      -2.040131    -1.396921    -2.201090      27.25
 C      -2.198419    -2.786112    -0.431309     109.44
 O      -2.950020    -3.855226    -1.161158     200.47
 H      -2.324773    -4.089114    -1.877941      29.98
 H      -2.640624    -2.737127     0.604090      26.20
 H      -1.090685    -3.010442    -0.391130      25.82
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 C       1.996088    -0.877381    -1.891878      26.45
 H       2.466291    -1.308874    -2.754975      17.83
 C       2.093857     0.306934     0.284994      64.89
 H       2.631419     0.769163     1.037091      22.67
 C       0.746463     0.131102     0.417506      23.64
 O       0.007406     0.550963     1.482319     222.07
 C       0.740413     1.168851     2.601937     119.72
 H       0.033860     1.552464     3.244283      27.63
 H       1.408078     0.445320     3.130672      26.68
 H       1.322084     1.927268     2.149918      27.63
 C      -0.025118    -0.426696    -0.632712      26.82
 O      -1.465866    -0.448873    -0.345290     165.91
 C       0.562515    -0.998883    -1.715120     109.22
 H       0.210385    -1.701197    -2.566217      21.01
 C       2.747198    -0.172872    -0.948650      30.24
 C       4.221614     0.063219    -1.117111     107.72
 H       4.556837    -0.069124    -2.184373      20.82
 O       4.506630     1.412846    -0.706661     251.81
 H       5.503176     1.646684    -0.977915      20.01
 C       5.132759    -0.847832    -0.251514      76.67
 H       5.036269    -0.552421     0.883564      23.35
 O       4.618732    -2.179491    -0.230100     325.50
 H       4.739879    -2.522970    -1.155617      29.33
 C       6.612043    -0.778140    -0.632034     113.01
 O       7.120200     0.618986    -0.691598     267.33
 H       6.970404     0.867903     0.290792      28.95
 H       6.830763    -1.024095    -1.644629      30.61
 H       7.095767    -1.336208     0.106694      29.91
55
name= lig-ACN-Water-frame_140
 C      -4.283999     0.438653    -3.162956      80.57
 H      -4.520584    -0.510405    -3.534453      30.09
 C      -3.690179     1.814786    -1.232043      76.00
 H      -3.513260     1.754056    -0.164124      22.59
 C      -3.690446     2.929125    -2.101566      11.17
 O      -3.291458     4.141907    -1.626583     202.03
 C      -2.520678     4.186664    -0.417583     110.87
 H      -1.739797     3.445977    -0.359032      28.68
 H      -3.153983     4.044310     0.401221      28.21
 H      -2.119299     5.357972    -0.323780      24.89
 C      -4.114301     2.835840    -3.465639       1.37
 O      -4.123276     4.039767    -4.370070      89.77
 H      -3.809662     4.895343    -3.802754      20.37
 C      -4.369603     1.584436    -4.036781      57.74
 H      -4.802485     1.414319    -4.965877      17.58
 C      -3.916310     0.540581    -1.827515      -3.44
 C      -3.763852    -0.765061    -0.945593      94.71
 H      -4.316262    -1.474724    -1.444597      27.31
 O      -4.293950    -0.700503     0.344644     236.29
 H      -3.763065    -0.246056     1.075129      23.19
 C      -2.357575    -1.331456    -1.074872      86.35
 H      -2.037638    -1.413244    -2.210602      27.54
 C      -2.270410    -2.754711    -0.422451     117.53
 O      -2.947653    -3.799985    -1.176733     200.36
 H      -2.422209    -4.089138    -2.022505      28.54
 H      -2.724891    -2.774213     0.555554      26.45
 H      -1.208538    -3.031165    -0.273308      26.99
 C       2.001160    -0.925603    -1.820453      45.02
 H       2.495546    -1.311531    -2.689150      24.74
 C       2.110549     0.365643     0.208162      64.89
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 H       2.676965     1.023656     0.916877      20.71
 C       0.688555     0.157570     0.344179      15.09
 O       0.020665     0.491676     1.526426     210.44
 C       0.782680     1.198028     2.566631     120.22
 H       0.113603     1.414688     3.272517      28.35
 H       1.551040     0.552610     2.999148      26.76
 H       1.191395     2.152340     2.278641      26.50
 C      -0.134785    -0.522540    -0.625108      26.57
 O      -1.410319    -0.527313    -0.311181     184.65
 C       0.591000    -1.071680    -1.730736      67.43
 H      -0.164401    -1.626557    -2.378817      20.00
 C       2.715380    -0.090871    -0.922695      38.94
 C       4.211448     0.122478    -1.139693      99.28
 H       4.388257    -0.086764    -2.209073      26.39
 O       4.481153     1.496476    -0.803729     226.01
 H       5.440730     1.500662    -0.722210      23.04
 C       5.068105    -0.774174    -0.244924      88.73
 H       4.973210    -0.272357     0.789788      24.83
 O       4.693402    -2.140198    -0.238666     336.11
 H       4.711532    -2.527932    -1.105311      31.21
 C       6.621362    -0.779659    -0.617184     105.28
 O       7.102073     0.659283    -0.603522     205.69
 H       7.362440     0.961034     0.395518      26.70
 H       6.747459    -1.299716    -1.527797      32.17
 H       7.235783    -1.338720     0.043840      30.66
55
name= lig-ACN-Water-frame_141
 C      -4.265419     0.442279    -3.158964      82.10
 H      -4.426364    -0.521345    -3.595361      23.12
 C      -3.693357     1.774661    -1.232308     104.52
 H      -3.440461     1.993861    -0.244662      22.35
 C      -3.697403     2.922896    -2.080566     -17.70
 O      -3.352428     4.207283    -1.691575     213.41
 C      -2.558206     4.211812    -0.462304     117.20
 H      -1.698222     3.466798    -0.533203      26.30
 H      -3.128863     4.105901     0.384363      28.13
 H      -2.033894     5.271346    -0.459542      25.21
 C      -4.091492     2.946768    -3.482815       2.42
 O      -4.110492     3.931681    -4.328673      70.96
 H      -3.921057     4.916425    -3.996104      19.10
 C      -4.393084     1.618140    -3.952722      34.19
 H      -4.516526     1.600601    -5.019845      25.31
 C      -3.920159     0.524798    -1.756167      22.09
 C      -3.756612    -0.699620    -0.991411      76.71
 H      -4.381871    -1.361014    -1.412753      27.61
 O      -4.263083    -0.672894     0.428269     160.70
 H      -3.425122    -0.365480     0.999597      22.81
 C      -2.332532    -1.412006    -1.061557      84.40
 H      -2.073092    -1.347027    -2.185284      28.89
 C      -2.322715    -2.784235    -0.411256     125.80
 O      -2.960637    -3.759910    -1.239766     224.93
 H      -2.294595    -3.897091    -1.964647      29.59
 H      -2.818731    -2.665700     0.493770      27.84
 H      -1.290877    -3.058750    -0.197586      26.97
 C       1.957944    -0.921644    -1.816358      35.24
 H       2.464420    -1.329155    -2.687923      19.61
 C       2.001250     0.475060     0.148900      75.56
 H       2.603960     1.164348     0.900486      19.08
 C       0.692708     0.202629     0.385246      20.53
 O       0.039772     0.483200     1.575671     232.97
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 C       0.789804     1.225429     2.559974     117.79
 H       0.194317     1.244493     3.358884      27.27
 H       1.701560     0.704724     2.791415      26.42
 H       1.027227     2.219526     2.167047      26.13
 C      -0.006629    -0.568978    -0.583743      33.48
 O      -1.465560    -0.580129    -0.290166     153.48
 C       0.570300    -1.169014    -1.709692      70.24
 H       0.239664    -1.660059    -2.612549      23.18
 C       2.708792    -0.134118    -0.969078      61.49
 C       4.169185     0.160091    -1.217166      98.92
 H       4.464735    -0.041165    -2.229936      23.53
 O       4.509404     1.586134    -0.890162     265.07
 H       5.425843     1.655464    -0.684711      22.78
 C       5.123648    -0.735273    -0.245149      93.38
 H       4.862811    -0.475380     0.790729      23.23
 O       4.719584    -2.163521    -0.205815     323.65
 H       4.833211    -2.496494    -1.125020      30.47
 C       6.592601    -0.675304    -0.551156     106.95
 O       7.109866     0.677391    -0.557021     332.87
 H       7.376404     0.783329     0.398768      31.15
 H       6.724115    -0.908710    -1.569747      32.00
 H       7.085196    -1.286591     0.211292      29.42
55
name= lig-ACN-Water-frame_142
 C      -4.277070     0.482916    -3.137179      18.75
 H      -4.521633    -0.468730    -3.657953      16.73
 C      -3.661207     1.882511    -1.256825      28.37
 H      -3.349092     1.886377    -0.257409      26.84
 C      -3.747301     3.013159    -2.074652      30.31
 O      -3.386763     4.278684    -1.691997     233.22
 C      -2.572987     4.304909    -0.517774     117.70
 H      -1.755268     3.445314    -0.582115      28.96
 H      -3.134052     4.093859     0.354534      26.93
 H      -2.146264     5.303728    -0.445561      26.64
 C      -4.069252     2.814830    -3.398115      -1.67
 O      -4.110362     3.903679    -4.349139     146.61
 H      -3.809621     4.723686    -3.840135      17.63
 C      -4.378672     1.609623    -3.931758     112.11
 H      -4.546266     1.489416    -5.028256      38.69
 C      -3.947983     0.548240    -1.795779     -61.78
 C      -3.803389    -0.837251    -0.955267      74.22
 H      -4.394332    -1.540459    -1.340935      30.08
 O      -4.211777    -0.634259     0.432950     141.99
 H      -3.503709    -0.210012     1.120088      23.40
 C      -2.349247    -1.399157    -1.047934      98.83
 H      -1.963365    -1.615818    -2.059977      30.29
 C      -2.348795    -2.823537    -0.375021     116.03
 O      -2.980542    -3.767954    -1.356842     170.47
 H      -2.377873    -4.052120    -2.028927      31.67
 H      -2.984991    -2.926408     0.449741      27.76
 H      -1.356433    -3.146266    -0.131248      27.69
 C       1.982829    -0.917850    -1.905815      30.00
 H       2.510275    -1.307314    -2.798977      19.35
 C       2.026864     0.572582     0.073909      57.65
 H       2.667071     1.309698     0.778131      19.38
 C       0.684909     0.159671     0.419920      18.25
 O       0.028109     0.495417     1.593214     214.45
 C       0.806450     1.265725     2.583036     115.91
 H       0.288441     1.256257     3.504174      26.98
 H       1.771647     0.897701     2.720129      26.96
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 H       0.802909     2.321337     2.264195      26.25
 C      -0.109536    -0.622803    -0.531137      22.76
 O      -1.407628    -0.591962    -0.283129     184.13
 C       0.593871    -1.187348    -1.645395      55.58
 H      -0.062153    -1.732528    -2.235197      25.22
 C       2.677539    -0.067642    -0.972982      52.78
 C       4.228483     0.179649    -1.206553      92.83
 H       4.414738    -0.033964    -2.213747      24.04
 O       4.513946     1.608636    -0.970278     263.83
 H       5.542967     1.669906    -0.831998      18.12
 C       5.031992    -0.749627    -0.236277     101.36
 H       4.916947    -0.287235     0.723847      24.69
 O       4.742872    -2.154084    -0.193555     310.95
 H       4.831052    -2.542010    -1.149269      26.51
 C       6.580089    -0.590030    -0.548282     107.72
 O       7.156594     0.750794    -0.483760     366.88
 H       7.205323     1.059657     0.384961      37.09
 H       6.790899    -1.072368    -1.481512      32.14
 H       7.177227    -1.286272     0.103624      29.06
55
name= lig-ACN-Water-frame_143
 C      -4.344050     0.403065    -3.124057      45.36
 H      -4.633442    -0.669781    -3.432980      27.09
 C      -3.637369     1.826953    -1.235429      65.85
 H      -3.312941     1.968550    -0.201797      24.14
 C      -3.772323     3.039851    -2.034120     -12.27
 O      -3.429853     4.361052    -1.684002     237.20
 C      -2.575086     4.416646    -0.505412     123.75
 H      -1.574162     3.738965    -0.601494      26.86
 H      -3.162291     4.193960     0.414530      26.94
 H      -2.268956     5.362906    -0.418954      28.57
 C      -4.090049     2.867309    -3.481266     -10.51
 O      -4.097610     3.881512    -4.319004      88.55
 H      -3.783236     4.741367    -3.996173      22.52
 C      -4.352986     1.527983    -4.011575      30.28
 H      -4.770621     1.456244    -5.085557      14.54
 C      -3.943577     0.555218    -1.754776      33.08
 C      -3.783797    -0.782203    -0.926508      74.73
 H      -4.392514    -1.480764    -1.331712      28.71
 O      -4.204524    -0.621132     0.413334     204.67
 H      -3.539108     0.004231     0.780827      28.11
 C      -2.353532    -1.487934    -0.966319      92.78
 H      -2.184837    -1.413556    -2.022571      30.89
 C      -2.404405    -2.935704    -0.420813     127.48
 O      -2.991416    -3.793759    -1.466477     187.25
 H      -2.223781    -3.999296    -2.085202      27.94
 H      -2.979390    -2.941396     0.501731      27.36
 H      -1.418687    -3.271946    -0.147385      27.42
 C       1.958447    -0.864842    -1.871647      13.56
 H       2.438831    -1.345449    -2.756622      17.75
 C       1.999216     0.558581     0.059757      54.96
 H       2.531669     1.385411     0.685482      23.63
 C       0.723731     0.160991     0.422852      23.74
 O       0.042292     0.530812     1.628997     220.37
 C       0.793134     1.334883     2.599878     122.67
 H       0.254205     1.081526     3.539322      26.38
 H       1.763254     0.971345     2.675566      28.44
 H       0.835143     2.414302     2.380950      26.86
 C      -0.014614    -0.605756    -0.485387      21.48
 O      -1.461400    -0.592746    -0.265027     129.62
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 C       0.595169    -1.180954    -1.591257      63.14
 H       0.172366    -1.845224    -2.234264      24.97
 C       2.698910     0.022759    -1.100848      38.18
 C       4.166565     0.170408    -1.211445     113.65
 H       4.490217    -0.154992    -2.144786      26.57
 O       4.526796     1.565959    -1.016222     247.88
 H       5.556543     1.658072    -1.123399      20.63
 C       5.065416    -0.673773    -0.209460      87.75
 H       4.770999    -0.447044     0.751732      26.91
 O       4.732994    -2.109186    -0.192645     304.53
 H       4.781118    -2.493471    -1.185356      26.53
 C       6.605592    -0.585042    -0.529902      95.08
 O       7.169807     0.851258    -0.450739     258.88
 H       7.452800     0.843271     0.436875      29.40
 H       6.750052    -0.820658    -1.575602      30.53
 H       7.127782    -1.176768     0.289278      27.81
55
name= lig-ACN-Water-frame_144
 C      -4.383305     0.397880    -3.091418      69.70
 H      -4.687340    -0.626486    -3.562881      29.54
 C      -3.638106     1.845355    -1.243263      55.89
 H      -3.283992     1.957478    -0.173484      21.99
 C      -3.761212     2.946781    -2.097616       0.18
 O      -3.478694     4.339367    -1.661232     195.42
 C      -2.604076     4.573016    -0.467821     116.30
 H      -1.590550     3.948835    -0.669913      26.49
 H      -3.040517     4.103129     0.502516      26.27
 H      -2.438956     5.529899    -0.420200      28.92
 C      -4.092863     2.780367    -3.460453       1.07
 O      -4.089557     3.943419    -4.364240      94.80
 H      -3.926283     4.728013    -3.814521      24.85
 C      -4.369637     1.496649    -3.962437      35.23
 H      -4.541288     1.368496    -5.100936      16.76
 C      -3.908962     0.518299    -1.754039     -23.03
 C      -3.740952    -0.714335    -0.936383      67.29
 H      -4.403303    -1.413102    -1.348629      23.97
 O      -4.236766    -0.581568     0.445152     175.15
 H      -3.636074    -0.291166     1.102053      26.44
 C      -2.375985    -1.476135    -0.981871      84.95
 H      -1.963109    -1.639024    -1.930336      28.38
 C      -2.424973    -3.023861    -0.483940     112.72
 O      -2.985606    -3.825002    -1.540707     179.08
 H      -2.329441    -4.043739    -2.328318      26.35
 H      -3.172849    -3.182293     0.359650      24.43
 H      -1.413709    -3.359737    -0.239805      26.02
 C       1.936415    -0.853943    -1.857416      33.86
 H       2.454336    -1.391173    -2.672389      21.10
 C       2.038538     0.569845     0.076257      63.11
 H       2.618763     1.250603     0.714455      22.08
 C       0.714162     0.231536     0.468978      27.62
 O       0.101457     0.594239     1.618288     237.85
 C       0.795974     1.346762     2.632417     118.61
 H       0.241165     1.260840     3.664285      24.70
 H       1.802711     1.059213     2.771270      26.83
 H       0.698280     2.399882     2.363017      25.39
 C      -0.099394    -0.606360    -0.461435      24.35
 O      -1.439372    -0.620441    -0.214601     141.43
 C       0.612067    -1.185447    -1.588299      62.25
 H       0.083545    -1.786644    -2.272064      24.37
 C       2.640645     0.090147    -1.088647      45.86
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 C       4.205466     0.154276    -1.269316      91.62
 H       4.401571    -0.161389    -2.239479      27.90
 O       4.536782     1.554106    -1.073176     247.92
 H       5.485560     1.607310    -1.005098      22.52
 C       5.073624    -0.654904    -0.175913      96.32
 H       4.978759    -0.202096     0.725466      28.10
 O       4.708956    -2.038122    -0.204762     323.06
 H       4.901268    -2.416781    -1.155396      27.00
 C       6.607059    -0.458801    -0.484255     103.97
 O       7.161211     0.865231    -0.438173     295.66
 H       7.425954     1.155962     0.489560      27.46
 H       6.824000    -0.897377    -1.488185      30.91
 H       7.213992    -1.249976     0.089165      28.64
55
name= lig-ACN-Water-frame_145
 C      -4.361660     0.410965    -3.057658      92.05
 H      -4.644753    -0.631594    -3.453409      28.25
 C      -3.624484     1.818597    -1.271078      72.20
 H      -3.332704     1.911175    -0.165109      22.32
 C      -3.683851     2.989932    -2.082831      -5.05
 O      -3.544623     4.223875    -1.636230     223.59
 C      -2.670714     4.566257    -0.513195     121.98
 H      -1.561610     4.186252    -0.621619      26.02
 H      -3.154561     4.257107     0.525151      25.32
 H      -2.476790     5.676645    -0.474612      25.44
 C      -4.066508     2.846543    -3.502934      13.57
 O      -4.094091     3.890661    -4.330975      70.72
 H      -3.831327     4.769573    -3.906342      22.58
 C      -4.401727     1.533174    -3.931921      32.89
 H      -4.583727     1.332421    -5.033653      20.40
 C      -3.880339     0.551466    -1.774656       5.39
 C      -3.738092    -0.774509    -0.885783      40.60
 H      -4.364209    -1.523055    -1.358513      24.46
 O      -4.291700    -0.563425     0.481020     178.79
 H      -3.505200    -0.344466     1.061735      25.13
 C      -2.325631    -1.485649    -0.990228      86.87
 H      -2.126519    -1.349376    -2.007642      29.44
 C      -2.437307    -3.003193    -0.551870     110.34
 O      -3.002593    -3.865598    -1.621874     191.21
 H      -2.260958    -4.060998    -2.288216      26.53
 H      -3.087517    -3.192103     0.427682      23.69
 H      -1.422541    -3.348221    -0.215410      24.61
 C       1.938977    -0.854471    -1.860697      24.94
 H       2.446700    -1.291349    -2.717870      18.55
 C       2.060018     0.622915     0.148606      52.87
 H       2.639040     1.134449     0.835034      22.14
 C       0.712102     0.255375     0.403284      11.08
 O       0.095686     0.636748     1.637771     193.73
 C       0.821389     1.412724     2.667481      94.22
 H       0.091560     1.178398     3.592298      22.77
 H       1.823328     0.997944     2.865430      25.00
 H       0.928986     2.472816     2.431909      25.67
 C      -0.060216    -0.556107    -0.465567      20.17
 O      -1.439722    -0.695666    -0.129817     169.82
 C       0.522497    -1.151106    -1.550108      57.06
 H      -0.089097    -1.821844    -2.197998      22.22
 C       2.684202     0.014020    -1.023174      36.76
 C       4.187524     0.186675    -1.260070     108.34
 H       4.472780    -0.162782    -2.197697      24.26
 O       4.559437     1.597766    -1.150669     299.48
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 H       5.454179     1.659257    -0.841049      18.86
 C       5.063077    -0.577542    -0.242108      97.48
 H       4.715952    -0.313592     0.675685      24.53
 O       4.703862    -1.973566    -0.178256     324.95
 H       4.865248    -2.424432    -1.035458      29.65
 C       6.629180    -0.470450    -0.493279      90.47
 O       7.150104     0.917808    -0.439472     349.69
 H       7.144608     1.022237     0.623748      25.77
 H       6.795710    -0.738183    -1.572432      29.29
 H       7.169575    -1.009599     0.346860      27.48
55
name= lig-ACN-Water-frame_146
 C      -4.315693     0.427961    -3.101459      28.20
 H      -4.647649    -0.566102    -3.497560      25.78
 C      -3.556495     1.805441    -1.247483      61.94
 H      -3.323781     2.058328    -0.173418      23.16
 C      -3.652306     2.906195    -2.084454      -0.09
 O      -3.587357     4.248006    -1.605357     259.93
 C      -2.719687     4.497771    -0.536758     107.29
 H      -1.815616     3.825892    -0.603222      26.70
 H      -3.215063     4.261715     0.528430      25.22
 H      -2.503322     5.683376    -0.706098      24.09
 C      -4.021100     2.819854    -3.431295       2.71
 O      -4.100035     3.895802    -4.342433      22.44
 H      -3.796940     4.784440    -3.862866      20.27
 C      -4.417648     1.572833    -3.943853      51.71
 H      -4.890403     1.567439    -4.925629      25.09
 C      -3.869771     0.469920    -1.699423     -62.25
 C      -3.782446    -0.780175    -0.860060      48.06
 H      -4.481859    -1.544655    -1.295515      23.16
 O      -4.298222    -0.590708     0.457045     149.32
 H      -3.664127    -0.091984     1.147607      25.12
 C      -2.356549    -1.445585    -0.955125      93.43
 H      -1.968873    -1.358460    -1.935598      30.72
 C      -2.396281    -2.976031    -0.626662     111.45
 O      -3.015252    -3.839976    -1.632426     193.75
 H      -2.350898    -4.117411    -2.271954      29.69
 H      -3.136563    -2.929689     0.320201      24.51
 H      -1.359348    -3.392456    -0.386522      25.36
 C       1.879900    -0.830663    -1.803482      46.55
 H       2.278845    -1.229807    -2.715287      23.84
 C       2.073072     0.563081     0.143111      66.19
 H       2.582391     1.195971     0.763247      22.13
 C       0.731425     0.352470     0.477409      28.92
 O       0.077438     0.678171     1.610282     217.51
 C       0.824977     1.414590     2.673022      99.23
 H       0.103885     1.503561     3.638800      23.44
 H       1.747709     0.801147     2.964878      24.75
 H       1.022210     2.453336     2.377449      25.38
 C      -0.074406    -0.497093    -0.432504      28.06
 O      -1.419090    -0.784516    -0.037118     167.36
 C       0.562973    -1.086721    -1.580628      54.31
 H       0.059875    -1.844505    -2.320333      22.00
 C       2.708903    -0.073616    -0.943524      45.89
 C       4.184888     0.240898    -1.273663      92.45
 H       4.318157    -0.092362    -2.264175      25.09
 O       4.547451     1.671967    -1.208757     237.65
 H       5.561458     1.655283    -0.979284      18.85
 C       5.059182    -0.548026    -0.250802     104.95
 H       5.016338    -0.067096     0.667044      25.57
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 O       4.707538    -1.964395    -0.161543     309.69
 H       4.764808    -2.298721    -1.056201      30.41
 C       6.592091    -0.455432    -0.498183      91.63
 O       7.100172     0.965399    -0.402861     277.17
 H       7.627334     1.190670     0.484055      26.96
 H       6.959131    -0.945346    -1.463998      31.30
 H       7.046266    -1.196903     0.207028      29.50
55
name= lig-ACN-Water-frame_147
 C      -4.284833     0.413333    -3.084058      47.86
 H      -4.670262    -0.490488    -3.514214      18.19
 C      -3.502166     1.741334    -1.189959      55.27
 H      -3.222213     1.762533    -0.136220      22.29
 C      -3.661433     2.917869    -2.044580      -9.78
 O      -3.652531     4.227717    -1.647810     234.65
 C      -2.720503     4.437722    -0.485933      95.66
 H      -1.881045     3.758985    -0.507675      28.24
 H      -3.311434     4.376265     0.534684      24.21
 H      -2.180413     5.548562    -0.494488      23.45
 C      -4.006016     2.807723    -3.457547      10.13
 O      -4.093747     3.910603    -4.301017     150.10
 H      -3.949143     4.816235    -3.791969      17.13
 C      -4.419472     1.551281    -3.907902      54.28
 H      -4.748390     1.409040    -4.905777      30.99
 C      -3.880627     0.510113    -1.771899      34.00
 C      -3.777432    -0.766341    -0.883539      82.90
 H      -4.433445    -1.600519    -1.376578      26.26
 O      -4.298280    -0.623479     0.480790     205.70
 H      -3.613733    -0.080445     0.957819      27.48
 C      -2.329046    -1.427043    -0.961729      86.37
 H      -2.011271    -1.224054    -1.985121      28.30
 C      -2.379378    -2.942453    -0.625261     111.17
 O      -3.048837    -3.771419    -1.614066     201.02
 H      -2.428039    -3.977876    -2.335472      29.75
 H      -2.880970    -3.346692     0.393535      24.44
 H      -1.268333    -3.259024    -0.443163      25.51
 C       1.951784    -0.814732    -1.805859      25.65
 H       2.433344    -1.237223    -2.676091      17.74
 C       2.098888     0.535141     0.218433      67.57
 H       2.708573     1.253559     0.712365      23.09
 C       0.670767     0.302671     0.452757      22.27
 O       0.035780     0.781415     1.651262     208.43
 C       0.805906     1.398548     2.649238      94.20
 H       0.016744     1.659921     3.479599      23.96
 H       1.698161     0.736080     3.089777      25.36
 H       1.306831     2.308361     2.235964      24.94
 C      -0.124156    -0.501858    -0.403526      36.04
 O      -1.379008    -0.829985     0.050504     169.39
 C       0.526616    -0.996579    -1.521628      77.03
 H      -0.149029    -1.616476    -2.281901      20.19
 C       2.695496    -0.025795    -0.930718      33.57
 C       4.168175     0.233997    -1.281309      84.13
 H       4.403998    -0.107075    -2.279609      26.56
 O       4.504060     1.707744    -1.240628     154.43
 H       5.531530     1.800665    -0.967491      20.24
 C       5.122855    -0.526260    -0.246148      90.47
 H       4.799240    -0.175610     0.709998      27.55
 O       4.710125    -1.926403    -0.160782     276.10
 H       4.759073    -2.355062    -1.074507      31.50
 C       6.618269    -0.432615    -0.489465      99.83
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 O       7.061568     0.951360    -0.401274     294.37
 H       7.414135     0.969857     0.506876      28.28
 H       6.822112    -0.721674    -1.570402      28.05
 H       7.157690    -0.932641     0.308861      28.90
55
name= lig-ACN-Water-frame_148
 C      -4.339158     0.367074    -3.091399      65.38
 H      -4.610006    -0.603379    -3.387289      26.69
 C      -3.509814     1.768157    -1.244000      70.18
 H      -3.159254     1.877186    -0.253892      22.21
 C      -3.706711     2.903154    -2.028765       8.30
 O      -3.602335     4.227598    -1.593769     252.91
 C      -2.754561     4.393827    -0.424538     103.77
 H      -2.002711     3.662417    -0.381306      28.64
 H      -3.413016     4.274475     0.524503      25.31
 H      -2.390318     5.543212    -0.601773      23.68
 C      -4.021990     2.804394    -3.415628      -2.91
 O      -4.095268     3.905280    -4.233720     162.21
 H      -3.786980     4.763856    -3.819314      20.23
 C      -4.361392     1.505399    -3.951854      53.69
 H      -4.521871     1.415000    -4.997936      27.68
 C      -3.844797     0.499638    -1.736335      24.03
 C      -3.730768    -0.764401    -0.906590      78.84
 H      -4.458607    -1.574386    -1.424920      23.31
 O      -4.244368    -0.636246     0.471014     233.03
 H      -3.603044    -0.263255     1.035565      27.79
 C      -2.338454    -1.427447    -0.893759      92.07
 H      -1.891341    -1.318947    -1.916191      27.04
 C      -2.302825    -2.959753    -0.586245     106.44
 O      -3.086081    -3.687416    -1.619004     190.37
 H      -2.384791    -3.931751    -2.343974      27.58
 H      -2.757674    -2.898831     0.511685      24.50
 H      -1.210230    -3.342893    -0.691153      25.06
 C       1.899868    -0.784443    -1.788589      38.79
 H       2.306653    -1.267775    -2.682054      20.77
 C       2.030111     0.535341     0.265815      59.84
 H       2.469521     1.148834     1.102044      21.14
 C       0.700248     0.298841     0.562427      26.28
 O      -0.016374     0.827793     1.601798     224.61
 C       0.843441     1.448765     2.657920     106.73
 H       0.153839     1.908041     3.425362      25.18
 H       1.385360     0.512349     3.190646      24.38
 H       1.493510     2.310992     2.310212      24.23
 C      -0.075460    -0.506284    -0.339012      20.25
 O      -1.419596    -0.844317     0.062093     173.36
 C       0.546611    -0.962641    -1.547363      67.37
 H      -0.032012    -1.570792    -2.362530      20.77
 C       2.701677     0.056886    -0.959307      32.69
 C       4.205951     0.236351    -1.230578      95.09
 H       4.395471    -0.195678    -2.248103      28.51
 O       4.453467     1.690373    -1.260884     169.55
 H       5.277151     1.787927    -0.733151      24.02
 C       5.066821    -0.537418    -0.215943      96.29
 H       4.943810    -0.115012     0.807117      27.59
 O       4.722965    -1.913245    -0.186590     259.57
 H       4.910508    -2.286560    -1.165382      28.41
 C       6.646377    -0.409120    -0.493313      99.20
 O       7.054435     0.981405    -0.384113     274.96
 H       7.166266     1.215024     0.521139      29.53
 H       6.873951    -0.802844    -1.534492      29.64
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 H       7.189340    -1.128071     0.086151      30.78
55
name= lig-ACN-Water-frame_149
 C      -4.343340     0.359870    -3.065230      54.01
 H      -4.617154    -0.551955    -3.530415      26.93
 C      -3.532733     1.794629    -1.259640      64.12
 H      -3.215286     1.910622    -0.254130      22.34
 C      -3.757237     2.928788    -2.050140      27.01
 O      -3.524685     4.202850    -1.550284     229.89
 C      -2.816837     4.384691    -0.327800     112.71
 H      -1.925384     3.830664    -0.304146      29.71
 H      -3.411407     4.253204     0.614273      25.84
 H      -2.407650     5.494561    -0.275224      24.94
 C      -4.071564     2.741226    -3.399336      12.77
 O      -4.102860     3.882770    -4.205391     201.40
 H      -3.692325     4.658414    -3.822175      24.30
 C      -4.257525     1.479463    -3.965549      46.02
 H      -4.578456     1.460255    -5.008557      16.38
 C      -3.840323     0.458752    -1.750387       7.98
 C      -3.686175    -0.790519    -0.851062      83.29
 H      -4.417469    -1.636474    -1.371418      22.20
 O      -4.189767    -0.652937     0.453920     216.09
 H      -3.491253    -0.148235     0.992497      25.06
 C      -2.250091    -1.466616    -0.913486      85.84
 H      -1.899673    -1.298992    -2.004186      26.13
 C      -2.269503    -2.941921    -0.589312     119.74
 O      -3.112393    -3.600936    -1.580358     208.39
 H      -2.542219    -4.062066    -2.284347      27.54
 H      -2.752834    -3.425590     0.342790      24.12
 H      -1.193587    -3.360452    -0.476343      25.53
 C       1.881111    -0.666881    -1.777873       3.79
 H       2.358962    -1.045340    -2.698773      19.90
 C       2.045956     0.552018     0.263126      91.48
 H       2.892595     1.072934     0.897625      20.64
 C       0.668890     0.250295     0.579719      27.43
 O      -0.008025     0.922861     1.623807     218.21
 C       0.803307     1.472025     2.693391     109.18
 H       0.135817     2.042871     3.290204      24.74
 H       1.436566     0.632377     3.333184      25.81
 H       1.619947     2.088665     2.167809      24.26
 C      -0.097773    -0.571360    -0.334032      38.76
 O      -1.403360    -0.766934     0.054714     183.90
 C       0.512086    -0.976050    -1.521557      77.11
 H      -0.035100    -1.633804    -2.221514      19.68
 C       2.635288     0.068551    -0.882678      48.15
 C       4.138797     0.248529    -1.179693      79.26
 H       4.398008    -0.175723    -2.220529      26.40
 O       4.446260     1.663141    -1.255194     224.44
 H       5.209453     1.899080    -0.789402      25.86
 C       5.122232    -0.532394    -0.174409      89.43
 H       4.916886    -0.187230     0.906554      25.32
 O       4.734276    -1.950424    -0.225393     278.18
 H       4.796689    -2.277247    -1.211364      27.64
 C       6.586128    -0.407757    -0.507902     106.82
 O       7.050739     1.037673    -0.349268     231.50
 H       7.456365     1.061677     0.576155      28.12
 H       6.787128    -0.607233    -1.574547      32.25
 H       7.151215    -0.969615     0.184833      31.10
55
name= lig-ACN-Water-frame_150
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 C      -4.254233     0.340806    -3.097674      79.34
 H      -4.608902    -0.642644    -3.423765      27.43
 C      -3.582771     1.708073    -1.214133      86.79
 H      -3.249575     1.804061    -0.173579      22.94
 C      -3.732029     2.898275    -1.974863     -25.08
 O      -3.486260     4.213848    -1.579391     193.06
 C      -2.815011     4.390047    -0.172664     114.32
 H      -1.882825     3.827868    -0.093650      28.12
 H      -3.518541     3.992284     0.519092      27.89
 H      -2.697014     5.441289    -0.136976      26.70
 C      -4.054505     2.793115    -3.415371       1.57
 O      -4.123365     3.840264    -4.251074     110.86
 H      -3.871774     4.703008    -3.818927      23.72
 C      -4.260544     1.470975    -3.924220      44.21
 H      -4.513215     1.256478    -5.009438      19.67
 C      -3.855779     0.463318    -1.750036      20.25
 C      -3.641668    -0.830052    -0.893244      59.79
 H      -4.368553    -1.727235    -1.373346      23.85
 O      -4.145851    -0.665985     0.498491     141.64
 H      -3.582117     0.011335     1.111894      22.50
 C      -2.233858    -1.444009    -0.901813      84.41
 H      -1.809365    -1.338667    -1.989715      26.63
 C      -2.264642    -3.019571    -0.555093     119.59
 O      -3.132136    -3.584298    -1.596837     203.36
 H      -2.533569    -3.918394    -2.247910      30.64
 H      -2.653532    -2.893970     0.481317      26.47
 H      -1.224086    -3.447882    -0.680526      26.19
 C       1.820111    -0.603591    -1.835042      38.99
 H       2.264946    -0.889066    -2.808214      23.31
 C       2.045322     0.544167     0.342426      54.40
 H       2.477429     1.340256     1.121836      17.19
 C       0.714674     0.311834     0.589434      20.95
 O       0.008927     0.932473     1.627435     226.46
 C       0.791145     1.525752     2.695079     108.12
 H       0.139154     2.127177     3.228865      27.15
 H       1.126224     0.626282     3.447400      24.59
 H       1.621831     2.252578     2.383423      24.44
 C      -0.042915    -0.534739    -0.283306      21.93
 O      -1.416284    -0.683507     0.020097     169.99
 C       0.507832    -1.032272    -1.495742      76.15
 H       0.008998    -1.591862    -2.214645      21.22
 C       2.647014     0.023366    -0.858694      41.80
 C       4.102189     0.236165    -1.113283      77.71
 H       4.242968    -0.251380    -2.171308      24.91
 O       4.440369     1.694900    -1.239232     190.31
 H       5.420149     1.725308    -0.895827      20.38
 C       5.044402    -0.560648    -0.190484      86.58
 H       4.846887    -0.318932     0.958681      24.69
 O       4.757520    -1.981463    -0.241380     303.35
 H       4.756636    -2.271661    -1.189248      28.69
 C       6.586490    -0.310869    -0.500893     103.24
 O       7.035941     1.033510    -0.322036     250.70
 H       7.269927     1.190806     0.733258      22.14
 H       6.693703    -0.669945    -1.530240      33.27
 H       7.150176    -1.024303     0.058928      31.95
55
name= lig-ACN-Water-frame_151
 C      -4.159575     0.303150    -3.098155      29.98
 H      -4.349434    -0.689547    -3.630073      20.82
 C      -3.623565     1.718412    -1.148844      58.34
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 H      -3.302334     1.776820    -0.060302      22.04
 C      -3.670058     2.868877    -1.977300       7.59
 O      -3.399044     4.213885    -1.514633     218.24
 C      -2.912647     4.332709    -0.160665     135.68
 H      -1.900611     3.855489    -0.078008      28.42
 H      -3.532021     4.003419     0.580458      29.44
 H      -2.748879     5.286968     0.044451      28.93
 C      -4.003538     2.733930    -3.343086      -4.43
 O      -4.143972     3.842874    -4.331092     125.97
 H      -3.876505     4.799622    -3.982378      18.25
 C      -4.313021     1.482239    -3.899864      47.73
 H      -4.484124     1.566324    -5.044083      24.64
 C      -3.847735     0.382509    -1.710578      -3.57
 C      -3.667331    -0.815856    -0.866810      62.79
 H      -4.421935    -1.685416    -1.354064      21.73
 O      -4.142883    -0.713583     0.502682     168.90
 H      -3.419687    -0.202645     1.049460      23.91
 C      -2.212949    -1.441347    -0.908276      86.05
 H      -1.811905    -1.316638    -2.004433      26.75
 C      -2.261376    -2.931889    -0.552729     118.96
 O      -3.148404    -3.626187    -1.590533     175.44
 H      -2.555064    -3.859539    -2.356940      28.53
 H      -2.740147    -3.301293     0.332833      27.38
 H      -1.308752    -3.492234    -0.487577      27.03
 C       1.827630    -0.609553    -1.804660      38.92
 H       2.181846    -0.873850    -2.807767      23.57
 C       2.071822     0.525726     0.375991      64.80
 H       2.796340     1.228117     0.968300      21.71
 C       0.698420     0.366375     0.608009      23.20
 O       0.018813     0.927845     1.615369     221.41
 C       0.715671     1.594240     2.754154     101.58
 H      -0.031562     2.161949     3.226453      26.74
 H       1.203820     0.737673     3.437793      25.25
 H       1.578342     2.185896     2.364795      25.73
 C      -0.042325    -0.496565    -0.294675      23.15
 O      -1.411871    -0.612378    -0.003874     165.95
 C       0.547911    -1.006271    -1.465595      55.17
 H      -0.063259    -1.529868    -2.093562      21.68
 C       2.615125     0.053956    -0.834121      35.67
 C       4.098439     0.230188    -1.164584      79.10
 H       4.374908    -0.160009    -2.240981      25.66
 O       4.444622     1.683057    -1.186048     182.28
 H       5.511631     1.809596    -1.076157      21.22
 C       4.998132    -0.589137    -0.164377      79.28
 H       4.769793    -0.153885     0.943300      26.08
 O       4.775192    -2.001866    -0.246024     288.79
 H       4.959501    -2.324826    -1.147386      29.37
 C       6.528307    -0.335996    -0.489220     102.42
 O       7.008188     1.046771    -0.296383     221.53
 H       7.109463     1.270576     0.766059      22.37
 H       6.725738    -0.435968    -1.532215      31.33
 H       7.144166    -1.016981     0.093164      31.79
55
name= lig-ACN-Water-frame_152
 C      -4.108862     0.318175    -3.105479      58.35
 H      -4.152368    -0.750504    -3.566119      25.15
 C      -3.644015     1.711767    -1.158947      78.02
 H      -3.526412     1.857098    -0.036000      19.82
 C      -3.602172     2.908583    -1.957585      16.43
 O      -3.344239     4.140347    -1.493611     210.08
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 C      -2.956121     4.262559    -0.121554     141.60
 H      -2.014587     3.671195     0.091971      25.61
 H      -3.727109     3.870638     0.418798      30.30
 H      -2.768622     5.230823     0.007529      28.03
 C      -3.995390     2.809504    -3.385569      16.35
 O      -4.136068     3.768816    -4.307431      63.93
 H      -3.833190     4.698335    -3.921370      21.19
 C      -4.281549     1.486050    -3.845093      53.84
 H      -4.696936     1.308758    -4.913525      22.79
 C      -3.828255     0.461450    -1.714425      15.30
 C      -3.696067    -0.876980    -0.821258      75.20
 H      -4.367566    -1.762989    -1.374182      22.11
 O      -4.169542    -0.779670     0.500268     214.58
 H      -3.556560    -0.278090     1.048246      26.07
 C      -2.270217    -1.407080    -0.905270      78.69
 H      -1.953859    -1.302900    -2.013082      26.54
 C      -2.309142    -2.964373    -0.580356     123.42
 O      -3.108314    -3.655917    -1.573497     222.39
 H      -2.535569    -3.918456    -2.404242      27.27
 H      -2.778128    -2.946461     0.342905      27.81
 H      -1.273209    -3.240532    -0.513365      27.58
 C       1.894944    -0.663135    -1.755724      31.09
 H       2.411844    -1.000997    -2.654617      15.36
 C       2.126049     0.528290     0.342557      42.63
 H       2.778438     0.947521     1.129784      21.75
 C       0.734499     0.353515     0.594927       9.51
 O      -0.040901     0.965266     1.690413     212.50
 C       0.644913     1.617832     2.752368     117.95
 H      -0.117561     2.179717     3.323177      24.95
 H       1.136896     0.894289     3.522460      24.90
 H       1.322188     2.382734     2.383496      24.93
 C      -0.068566    -0.419709    -0.300443      21.43
 O      -1.409342    -0.591845    -0.026936     165.42
 C       0.508985    -0.942677    -1.442353      82.93
 H       0.070603    -1.604131    -2.173256      23.63
 C       2.668409     0.102783    -0.907638      32.10
 C       4.112430     0.247601    -1.209177      90.58
 H       4.259171    -0.182685    -2.307440      26.69
 O       4.440985     1.663510    -1.116090     223.80
 H       5.433982     1.677676    -0.991100      21.90
 C       5.034024    -0.559091    -0.199092      81.97
 H       4.702008    -0.352162     0.940894      24.75
 O       4.774011    -2.012434    -0.207397     295.82
 H       4.907036    -2.261749    -1.155827      29.29
 C       6.491088    -0.355988    -0.469839     103.56
 O       6.940633     1.063689    -0.276489     246.55
 H       7.485693     1.081854     0.625044      22.90
 H       6.558263    -0.703297    -1.477223      32.20
 H       7.091408    -1.039063     0.164203      30.21
55
name= lig-ACN-Water-frame_153
 C      -4.061651     0.350525    -3.038858      45.80
 H      -4.340430    -0.660019    -3.536413      24.53
 C      -3.650147     1.764910    -1.181048      67.84
 H      -3.553811     1.862081    -0.095496      21.86
 C      -3.615878     2.848737    -2.036413      23.59
 O      -3.278123     4.141002    -1.526728     173.65
 C      -2.990960     4.164453    -0.033539     108.24
 H      -2.151349     3.477193     0.288005      26.73
 H      -3.812175     4.037162     0.602947      28.46
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 H      -2.689712     5.175278     0.183710      27.28
 C      -3.984540     2.713671    -3.344873      18.91
 O      -4.107077     3.793482    -4.280888      57.81
 H      -4.027366     4.750136    -3.933579      19.47
 C      -4.232975     1.469658    -3.860621      54.60
 H      -4.564223     1.431976    -4.937693      21.25
 C      -3.830209     0.426663    -1.666455       1.69
 C      -3.736989    -0.817221    -0.895515      58.06
 H      -4.454141    -1.647509    -1.411962      21.66
 O      -4.242939    -0.839649     0.540388     117.90
 H      -3.854695    -0.081004     0.961423      28.45
 C      -2.299261    -1.415836    -0.961245      86.44
 H      -1.920942    -1.222395    -1.999852      26.13
 C      -2.293660    -2.914231    -0.563687     127.32
 O      -3.060303    -3.697627    -1.566368     239.64
 H      -2.367509    -3.990793    -2.183710      29.19
 H      -2.754744    -3.126037     0.326697      27.85
 H      -1.390504    -3.455971    -0.503188      27.18
 C       1.897368    -0.725585    -1.746718      37.51
 H       2.231554    -1.304533    -2.598113      21.79
 C       2.089933     0.558659     0.353382      57.15
 H       2.632512     1.051489     1.087420      23.52
 C       0.708914     0.390749     0.651162      10.40
 O      -0.054001     0.928326     1.679833     215.93
 C       0.595135     1.693255     2.782243     111.88
 H      -0.272864     2.093411     3.420099      23.81
 H       1.203532     0.947098     3.356832      25.23
 H       1.248171     2.450609     2.433489      25.85
 C      -0.088872    -0.352961    -0.344171       1.19
 O      -1.457975    -0.608082    -0.027584     135.17
 C       0.572721    -0.916501    -1.502514      59.05
 H      -0.140881    -1.546222    -2.138507      21.58
 C       2.689304     0.091389    -0.892478      41.38
 C       4.179530     0.255078    -1.184849      99.52
 H       4.477982    -0.071318    -2.279539      25.11
 O       4.462167     1.673550    -1.058294     227.96
 H       5.327136     1.748607    -0.720943      20.87
 C       4.984312    -0.590757    -0.203631      78.49
 H       4.801301    -0.029525     0.846602      23.10
 O       4.760090    -1.993325    -0.188373     281.66
 H       4.839476    -2.373863    -1.140387      27.81
 C       6.540459    -0.364119    -0.442008      99.35
 O       6.883101     1.018664    -0.312756     338.45
 H       7.132842     1.327734     0.625747      27.10
 H       6.957464    -0.604553    -1.412519      28.48
 H       7.109167    -1.001051     0.297593      28.31
55
name= lig-ACN-Water-frame_154
 C      -4.114081     0.301577    -3.057589      43.20
 H      -4.354518    -0.737317    -3.428743      23.84
 C      -3.638122     1.725843    -1.117626      76.45
 H      -3.370354     1.876402    -0.129576      20.51
 C      -3.618365     2.890029    -1.974265       9.79
 O      -3.206431     4.128148    -1.482256     184.69
 C      -3.032336     4.131724    -0.026649      98.04
 H      -2.380361     3.287392     0.220993      25.69
 H      -4.031086     4.039384     0.403583      26.27
 H      -2.371801     5.068283     0.159577      24.16
 C      -3.968226     2.768633    -3.418538       6.73
 O      -4.087917     3.803496    -4.245833     104.96
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 H      -3.875073     4.636756    -3.792569      23.75
 C      -4.173749     1.411992    -3.937176      60.16
 H      -4.317990     1.283493    -4.998594      23.13
 C      -3.869522     0.488120    -1.654801      28.98
 C      -3.807568    -0.840622    -0.838339      70.13
 H      -4.484979    -1.579827    -1.434912      23.08
 O      -4.308699    -0.842452     0.483517     171.55
 H      -3.772404    -0.174500     1.083709      23.76
 C      -2.274773    -1.423191    -0.966555      81.86
 H      -1.975643    -1.407681    -2.008277      26.29
 C      -2.260998    -2.934366    -0.541577     120.11
 O      -3.011787    -3.736605    -1.568735     240.88
 H      -2.460814    -4.089770    -2.262601      29.04
 H      -2.775074    -2.964278     0.362961      27.66
 H      -1.237722    -3.062520    -0.358156      27.28
 C       1.929886    -0.761561    -1.746636      25.54
 H       2.506801    -1.121102    -2.596754      13.38
 C       2.033842     0.611145     0.330425      63.50
 H       2.612607     1.309205     0.752228      19.90
 C       0.637885     0.401134     0.562002      14.68
 O      -0.043681     0.907133     1.690132     209.21
 C       0.574196     1.694935     2.772376     104.82
 H      -0.350755     2.028558     3.421677      22.87
 H       1.257615     1.140116     3.379447      26.97
 H       0.990283     2.577730     2.364143      25.68
 C      -0.134997    -0.360453    -0.372194      35.98
 O      -1.455408    -0.619701    -0.055453     192.17
 C       0.489077    -0.888194    -1.469316      91.79
 H      -0.026405    -1.537059    -2.306756      21.56
 C       2.639844    -0.001959    -0.822263      31.50
 C       4.174745     0.272601    -1.148804      68.89
 H       4.351513    -0.054586    -2.259336      21.40
 O       4.485821     1.715509    -0.994875     207.92
 H       5.392454     1.743380    -0.662784      20.15
 C       5.111574    -0.582936    -0.194972      81.55
 H       4.775898    -0.367120     0.909594      24.32
 O       4.702115    -1.988418    -0.170819     292.66
 H       4.948987    -2.306299    -1.134242      28.92
 C       6.596589    -0.408528    -0.372554      95.15
 O       6.860509     1.058446    -0.320497     298.12
 H       7.125846     1.224167     0.584501      30.19
 H       6.806520    -0.849715    -1.368389      31.95
 H       7.149880    -0.927594     0.481795      29.50
55
name= lig-ACN-Water-frame_155
 C      -4.191729     0.301719    -3.075226      52.87
 H      -4.272606    -0.691430    -3.494984      22.01
 C      -3.620021     1.745150    -1.131259      62.94
 H      -3.400108     1.719660    -0.111527      21.40
 C      -3.628058     2.869851    -1.951359      17.23
 O      -3.159961     4.106271    -1.473454     219.22
 C      -3.029160     4.134993    -0.061434      99.79
 H      -2.542413     3.313135     0.443158      26.94
 H      -4.007129     4.294585     0.506583      24.82
 H      -2.510707     5.176504     0.277039      24.01
 C      -3.914294     2.696262    -3.350746       4.04
 O      -4.072057     3.819691    -4.253121     152.55
 H      -3.819446     4.745759    -4.027690      21.74
 C      -4.087907     1.418318    -3.939013      59.29
 H      -4.289990     1.300534    -4.949274      24.43
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 C      -3.960925     0.432036    -1.693911       4.89
 C      -3.778053    -0.877426    -0.887618      81.02
 H      -4.362591    -1.713290    -1.360406      24.05
 O      -4.353746    -0.793266     0.465035     168.51
 H      -3.601047    -0.424592     1.131593      22.64
 C      -2.377856    -1.436299    -0.939171      95.73
 H      -2.084355    -1.222886    -1.925116      27.62
 C      -2.237874    -2.923519    -0.542799     128.92
 O      -2.936522    -3.763829    -1.515884     224.26
 H      -2.214435    -3.908503    -2.226517      26.59
 H      -2.753681    -3.134808     0.372497      27.07
 H      -1.320717    -3.442950    -0.483024      26.21
 C       1.870953    -0.751683    -1.679139      55.70
 H       2.200606    -1.147726    -2.644060      22.98
 C       1.978377     0.667385     0.233195      64.63
 H       2.340916     1.352616     0.908121      20.55
 C       0.620049     0.449626     0.532098      25.55
 O      -0.060569     0.862052     1.677652     228.21
 C       0.550451     1.698402     2.697426     113.86
 H      -0.324457     1.953817     3.417927      23.92
 H       1.293899     1.177456     3.187507      27.94
 H       0.959258     2.631236     2.319981      26.56
 C      -0.133266    -0.409602    -0.377103      18.39
 O      -1.490540    -0.621302    -0.086094     169.78
 C       0.526151    -0.932853    -1.559931      45.50
 H      -0.143860    -1.494124    -2.317657      20.83
 C       2.700201    -0.014439    -0.763486      50.16
 C       4.130412     0.293253    -1.046333      87.75
 H       4.318813    -0.023051    -2.132813      24.45
 O       4.440780     1.721785    -0.955806     192.40
 H       5.451322     1.787895    -0.680826      17.23
 C       5.084861    -0.609732    -0.099262      89.50
 H       4.921801    -0.138263     0.934105      24.37
 O       4.692849    -2.000284    -0.209887     280.45
 H       4.793027    -2.322179    -1.171511      28.72
 C       6.627078    -0.417549    -0.303771     100.23
 O       6.920882     1.057382    -0.312179     230.34
 H       7.301174     1.410479     0.495063      30.39
 H       7.082136    -0.791237    -1.291092      31.22
 H       7.269045    -0.935836     0.491177      30.10
55
name= lig-ACN-Water-frame_156
 C      -4.214934     0.301337    -3.108190      51.36
 H      -4.475780    -0.586162    -3.609388      20.90
 C      -3.675155     1.605938    -1.192047      68.19
 H      -3.482350     1.792312    -0.117379      18.36
 C      -3.581830     2.815578    -1.964909      24.22
 O      -3.147981     4.066877    -1.504420     202.70
 C      -3.045975     4.246240     0.020762      81.64
 H      -2.400024     3.457717     0.387383      24.54
 H      -4.140894     4.238951     0.414389      24.49
 H      -2.318954     5.237183     0.028530      22.90
 C      -3.859781     2.762176    -3.344710      13.47
 O      -4.050499     3.728833    -4.258166     175.39
 H      -3.819164     4.586795    -3.849562      24.10
 C      -4.066914     1.469454    -3.891039      82.00
 H      -4.229592     1.536124    -4.916183      26.17
 C      -3.998137     0.378207    -1.707447      42.56
 C      -3.841530    -0.884483    -0.912883      80.23
 H      -4.434462    -1.616230    -1.460486      23.23
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 O      -4.374289    -0.755267     0.458473     208.35
 H      -3.682341    -0.335424     1.063910      22.64
 C      -2.334027    -1.426121    -0.942297      80.93
 H      -2.033739    -1.465212    -1.940889      25.91
 C      -2.240709    -2.976356    -0.520764     112.56
 O      -2.887604    -3.800533    -1.491353     263.68
 H      -2.349660    -4.035985    -2.340777      25.67
 H      -2.671091    -3.119736     0.494738      24.87
 H      -1.173346    -2.932988    -0.379274      25.25
 C       1.917356    -0.746822    -1.693124      28.66
 H       2.538149    -1.219080    -2.477838      19.00
 C       1.924525     0.748792     0.273874      81.76
 H       2.670556     1.270358     0.885370      19.25
 C       0.570752     0.396324     0.475283      13.93
 O      -0.116406     0.819134     1.617165     203.55
 C       0.561664     1.683421     2.608524     107.45
 H      -0.222506     1.960010     3.351728      24.65
 H       1.307277     1.184053     3.060454      27.19
 H       0.963156     2.596506     2.091664      25.04
 C      -0.164644    -0.454666    -0.405394      22.37
 O      -1.525502    -0.592763    -0.074368     191.11
 C       0.475979    -0.948463    -1.518392      69.99
 H      -0.002869    -1.498504    -2.329744      20.46
 C       2.622581     0.050121    -0.795179      41.71
 C       4.191825     0.260267    -0.981550      79.72
 H       4.492865    -0.106304    -2.012702      22.43
 O       4.362291     1.706695    -0.921966     189.97
 H       5.353499     1.872566    -0.581752      17.95
 C       5.045162    -0.593781    -0.036873      96.47
 H       4.739423    -0.490277     1.021748      23.79
 O       4.714170    -1.997119    -0.238054     334.86
 H       4.809870    -2.170548    -1.190735      27.58
 C       6.647873    -0.359780    -0.257335      86.12
 O       7.030199     1.023744    -0.307273     314.53
 H       7.126672     1.182268     0.698823      27.74
 H       6.879267    -0.858098    -1.294015      30.05
 H       7.116957    -0.906203     0.623370      28.58
55
name= lig-ACN-Water-frame_157
 C      -4.219593     0.296745    -3.178899      42.12
 H      -4.593546    -0.574831    -3.629222      24.88
 C      -3.701346     1.623739    -1.186296      63.65
 H      -3.538711     1.579868    -0.054391      19.15
 C      -3.513031     2.777360    -1.942238      29.93
 O      -3.160855     4.033789    -1.450766     220.16
 C      -3.019730     4.316546    -0.064388     105.54
 H      -2.432153     3.623335     0.554091      26.97
 H      -4.049626     4.365608     0.584467      25.22
 H      -2.686813     5.478044     0.133942      24.41
 C      -3.832036     2.695795    -3.345975      19.84
 O      -4.005277     3.738978    -4.272071     147.73
 H      -3.713160     4.715740    -4.125988      18.36
 C      -4.119030     1.474403    -3.899652      38.86
 H      -4.318499     1.346562    -4.949428      23.72
 C      -4.005033     0.331370    -1.785203      17.83
 C      -3.894947    -0.932086    -0.895286      87.73
 H      -4.457509    -1.744043    -1.218575      25.57
 O      -4.384081    -0.742130     0.434261     203.08
 H      -3.930480    -0.082068     0.931364      27.69
 C      -2.389587    -1.483116    -0.952709      88.56
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 H      -2.017569    -1.288689    -1.915901      25.75
 C      -2.177977    -2.899477    -0.477851     118.85
 O      -2.872879    -3.863851    -1.459387     243.75
 H      -2.185178    -4.063327    -2.101395      28.85
 H      -2.775849    -3.142376     0.469270      23.96
 H      -1.208061    -3.408648    -0.427700      24.38
 C       1.912993    -0.750604    -1.698276      10.52
 H       2.417504    -1.347344    -2.484920      17.17
 C       1.937979     0.688420     0.258074      60.96
 H       2.266337     1.471753     1.053356      13.46
 C       0.569965     0.379614     0.510670      36.51
 O      -0.195259     0.806200     1.577402     236.31
 C       0.566052     1.633386     2.483951     124.17
 H      -0.133688     1.994822     3.186609      25.36
 H       1.312837     1.142006     2.954013      29.03
 H       0.955598     2.558804     1.935150      25.51
 C      -0.194060    -0.425621    -0.417370      20.45
 O      -1.547921    -0.579798    -0.089916     153.03
 C       0.540440    -0.998824    -1.540748      65.00
 H       0.043307    -1.642256    -2.176852      20.23
 C       2.600783     0.148603    -0.842140      53.09
 C       4.111515     0.246972    -0.965275      90.19
 H       4.397851    -0.092428    -1.982223      26.44
 O       4.340630     1.693201    -0.882283     176.16
 H       5.129286     1.896187    -0.385084      21.62
 C       5.054972    -0.589777     0.029205      93.92
 H       4.799119    -0.337206     1.024341      27.37
 O       4.761786    -1.993566    -0.280498     303.58
 H       5.035168    -2.206825    -1.211156      29.00
 C       6.532210    -0.376540    -0.189112      97.64
 O       7.097230     0.986474    -0.275456     281.61
 H       7.687465     1.376385     0.497258      27.20
 H       6.801182    -0.901196    -1.233206      30.70
 H       7.188429    -0.961826     0.513465      28.74
55
name= lig-ACN-Water-frame_158
 C      -4.247067     0.225128    -3.183725      47.13
 H      -4.415955    -0.727360    -3.677690      23.81
 C      -3.691692     1.568109    -1.172970      66.63
 H      -3.508547     1.750311    -0.061143      18.42
 C      -3.508478     2.766216    -1.939377      12.62
 O      -3.178367     4.025465    -1.444585     214.39
 C      -3.057532     4.366046    -0.045625      94.39
 H      -2.180778     3.814074     0.406681      24.94
 H      -4.168528     4.208785     0.425173      23.56
 H      -2.647794     5.456330    -0.204573      23.46
 C      -3.803556     2.697155    -3.371112      -3.14
 O      -3.932753     3.792746    -4.291925     132.98
 H      -3.610800     4.624092    -3.754364      20.77
 C      -4.199936     1.416056    -4.001111      70.34
 H      -4.521561     1.590585    -5.078962      19.08
 C      -3.986466     0.332914    -1.780595      30.48
 C      -3.892382    -0.979216    -0.917279      74.41
 H      -4.473556    -1.664984    -1.367542      25.38
 O      -4.418002    -0.744445     0.455446     158.53
 H      -3.869750     0.034658     0.785505      26.44
 C      -2.386662    -1.450097    -0.959015      82.66
 H      -2.222409    -1.473252    -2.027005      26.46
 C      -2.221587    -2.987774    -0.484142     115.22
 O      -2.861486    -3.885572    -1.375240     274.23
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 H      -2.301902    -4.202578    -2.096471      27.63
 H      -2.657330    -2.953314     0.598842      24.36
 H      -1.091096    -3.017690    -0.256854      23.77
 C       1.894010    -0.749372    -1.695948      29.58
 H       2.408476    -1.180855    -2.576730      14.32
 C       1.856191     0.633061     0.275736     130.43
 H       2.611492     1.405068     0.797906      19.90
 C       0.518373     0.329421     0.465874      18.37
 O      -0.233117     0.817926     1.548519     233.37
 C       0.534819     1.641807     2.440139     105.82
 H      -0.088621     1.981044     3.165333      26.82
 H       1.285902     1.039217     2.818925      27.43
 H       1.049378     2.471226     1.863963      23.67
 C      -0.168090    -0.431332    -0.475075      23.90
 O      -1.559345    -0.587703    -0.138290     172.95
 C       0.512727    -1.049717    -1.498111      69.40
 H       0.092832    -1.731727    -2.110901      20.28
 C       2.591816     0.088018    -0.846896      86.08
 C       4.079070     0.315674    -0.983246      92.16
 H       4.353186    -0.004199    -1.981015      26.38
 O       4.383892     1.713871    -0.843502     227.43
 H       4.935254     1.849470    -0.078080      26.25
 C       4.945686    -0.564925     0.008411      97.92
 H       4.631769    -0.445454     0.980348      29.26
 O       4.829777    -1.992891    -0.264414     261.76
 H       5.037544    -2.093150    -1.283295      26.87
 C       6.565796    -0.399767    -0.178320      83.29
 O       7.098555     0.944727    -0.299414     281.08
 H       7.371825     1.086994     0.690598      27.54
 H       6.750714    -0.837364    -1.269974      30.76
 H       6.971137    -1.050219     0.637999      29.01
55
name= lig-ACN-Water-frame_159
 C      -4.243184     0.249275    -3.169814      32.42
 H      -4.461823    -0.764602    -3.609176      25.52
 C      -3.644583     1.591700    -1.211871      62.06
 H      -3.465150     1.604333    -0.138252      20.71
 C      -3.580526     2.722593    -2.026290      21.26
 O      -3.209005     4.009440    -1.541054     186.14
 C      -3.078692     4.381831    -0.071335      95.21
 H      -2.248551     3.809132     0.478099      24.71
 H      -4.020676     4.173301     0.698718      23.43
 H      -2.996063     5.484002     0.030661      24.46
 C      -3.858679     2.661018    -3.457633      17.21
 O      -3.812276     3.775506    -4.205734      87.75
 H      -3.697170     4.756044    -3.872949      15.33
 C      -4.231203     1.443932    -3.958153      79.60
 H      -4.516713     1.257328    -5.068429      19.17
 C      -3.980956     0.309543    -1.787252      21.27
 C      -3.875052    -0.920926    -0.938863     101.15
 H      -4.402954    -1.684340    -1.292574      27.77
 O      -4.433128    -0.775871     0.426917     151.25
 H      -3.826243    -0.167197     1.095037      22.67
 C      -2.418111    -1.525709    -0.985220      88.93
 H      -1.945407    -1.460088    -1.975768      24.44
 C      -2.236491    -2.913527    -0.429328     119.22
 O      -2.890260    -3.941946    -1.269593     208.55
 H      -2.271570    -4.100924    -2.079188      27.16
 H      -2.753942    -3.232685     0.544858      24.29
 H      -1.111961    -3.269598    -0.447560      23.00
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 C       1.862761    -0.803555    -1.760130      27.84
 H       2.421415    -1.155143    -2.640631      19.74
 C       1.869961     0.595876     0.251916      66.21
 H       2.326407     1.215553     1.126435      15.66
 C       0.477477     0.361814     0.449192      25.32
 O      -0.267365     0.846406     1.498498     221.16
 C       0.542447     1.653948     2.466811     122.19
 H      -0.124577     2.041313     3.140980      26.32
 H       1.280735     1.102292     3.004467      27.05
 H       0.928667     2.549165     1.960074      25.61
 C      -0.251484    -0.505844    -0.467197      28.07
 O      -1.567174    -0.610412    -0.239313     195.03
 C       0.496905    -1.126215    -1.533981      74.42
 H      -0.026258    -1.690478    -2.260185      20.64
 C       2.534885    -0.008537    -0.795143      61.83
 C       4.089768     0.331573    -1.007359      76.41
 H       4.378497     0.184061    -2.006442      23.67
 O       4.451650     1.773161    -0.805209     195.24
 H       4.698340     2.114976     0.168018      22.57
 C       4.941408    -0.565674    -0.079742     106.92
 H       4.615289    -0.364837     0.869989      26.55
 O       4.857347    -1.995368    -0.258446     273.32
 H       4.777985    -2.265491    -1.248067      26.87
 C       6.489232    -0.402754    -0.216975     101.34
 O       7.089349     0.883533    -0.266171     314.88
 H       7.242543     1.311371     0.571992      30.53
 H       6.812213    -1.071788    -1.142919      30.09
 H       7.003508    -0.919836     0.615816      28.41
55
name= lig-ACN-Water-frame_160
 C      -4.250393     0.282411    -3.137407      48.56
 H      -4.670291    -0.652554    -3.656613      25.87
 C      -3.618917     1.592448    -1.264736      72.14
 H      -3.306474     1.717102    -0.276033      21.29
 C      -3.625065     2.756375    -2.030505      23.78
 O      -3.261039     4.023030    -1.589329     235.59
 C      -3.140639     4.309239    -0.158649     105.86
 H      -2.131301     3.907172     0.250518      24.92
 H      -4.174108     3.878060     0.267958      24.19
 H      -3.034005     5.340037    -0.200820      25.99
 C      -3.911807     2.673666    -3.388509       8.63
 O      -3.710197     3.777766    -4.223489      74.17
 H      -3.489588     4.496842    -3.594653      21.26
 C      -4.245854     1.388357    -3.963767      92.02
 H      -4.392263     1.347092    -5.101405      17.99
 C      -3.953793     0.351448    -1.777000      40.61
 C      -3.865415    -0.959305    -0.944168      82.86
 H      -4.500753    -1.568133    -1.421408      25.90
 O      -4.420044    -0.819163     0.388620     195.81
 H      -3.696471    -0.430269     1.009553      23.73
 C      -2.413701    -1.546567    -1.014035      89.59
 H      -2.389476    -1.661630    -2.139341      26.55
 C      -2.260075    -2.974812    -0.370836     112.46
 O      -2.955698    -3.994657    -1.204540     182.33
 H      -2.374921    -4.138621    -2.043688      26.76
 H      -2.583118    -2.762945     0.690462      25.78
 H      -1.090125    -3.180768    -0.205599      24.62
 C       1.843270    -0.851524    -1.754979      44.88
 H       2.272185    -1.335659    -2.636117      19.20
 C       1.812425     0.521192     0.288283      87.69
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 H       2.405401     1.087979     1.008411      21.71
 C       0.442585     0.337176     0.399933      12.78
 O      -0.251543     0.925624     1.505080     223.57
 C       0.466742     1.687518     2.502991     109.00
 H      -0.292699     1.984475     3.189941      25.64
 H       1.218380     1.009545     2.970481      26.12
 H       1.014763     2.475958     2.066189      27.06
 C      -0.193482    -0.569240    -0.497614      39.22
 O      -1.629703    -0.615934    -0.270986     165.09
 C       0.457058    -1.139720    -1.588014      39.75
 H      -0.078420    -1.750696    -2.370612      17.27
 C       2.602950    -0.024373    -0.841994      48.47
 C       4.064548     0.344347    -1.017152      97.86
 H       4.241710     0.222266    -2.025134      26.20
 O       4.444251     1.791788    -0.796477     238.28
 H       4.439052     2.010722     0.175159      27.70
 C       5.012728    -0.566081    -0.138619      98.39
 H       4.771607    -0.330720     0.835511      27.93
 O       4.785155    -2.033554    -0.269288     258.47
 H       4.908023    -2.172938    -1.244110      29.46
 C       6.503899    -0.436728    -0.202135     102.68
 O       7.094100     0.899064    -0.275358     276.55
 H       7.586671     0.964593     0.560212      29.52
 H       6.833896    -0.880586    -1.214105      30.29
 H       6.784584    -1.082206     0.645022      29.84
55
name= lig-ACN-Water-frame_161
 C      -4.326432     0.247729    -3.141327      39.72
 H      -4.602495    -0.801218    -3.523743      21.04
 C      -3.567665     1.632984    -1.182222      59.54
 H      -3.225472     1.674341    -0.190814      21.12
 C      -3.652307     2.782686    -2.014965      11.20
 O      -3.303032     4.057053    -1.662268     226.13
 C      -3.214636     4.246595    -0.285324     111.43
 H      -2.305139     3.723206     0.196459      26.05
 H      -4.059897     3.831548     0.416056      25.55
 H      -3.259854     5.222159    -0.068837      26.99
 C      -3.920603     2.687960    -3.434194      10.49
 O      -3.634675     3.734612    -4.238737     106.46
 H      -3.542030     4.653301    -3.948234      16.07
 C      -4.217468     1.456806    -3.987685      80.53
 H      -4.441009     1.441965    -5.055922      27.70
 C      -3.924558     0.332707    -1.771557      16.64
 C      -3.918574    -0.991980    -1.000436      87.38
 H      -4.492450    -1.717500    -1.458770      26.56
 O      -4.381582    -0.889656     0.379628     179.99
 H      -3.805779    -0.392844     0.927917      27.20
 C      -2.482945    -1.611315    -1.046574      86.42
 H      -1.925248    -1.576736    -2.046627      24.46
 C      -2.298706    -2.985001    -0.353382     119.39
 O      -3.013152    -4.012956    -1.096656     201.84
 H      -2.462384    -4.320814    -1.814310      31.17
 H      -2.874198    -3.170064     0.549563      25.43
 H      -1.158553    -3.277927    -0.237937      25.17
 C       1.875706    -0.885271    -1.735896      12.42
 H       2.512217    -1.291965    -2.517350      14.53
 C       1.873812     0.439038     0.248538      82.06
 H       2.330546     1.110971     0.857837      17.04
 C       0.466397     0.293462     0.452121      37.68
 O      -0.283849     0.963870     1.430016     224.07
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 C       0.430419     1.669107     2.531282     108.51
 H      -0.354926     2.129418     3.204612      24.03
 H       1.046507     0.941292     3.163108      25.09
 H       0.938863     2.505743     2.216353      25.87
 C      -0.285485    -0.536402    -0.494179      42.90
 O      -1.611002    -0.622355    -0.323146     187.62
 C       0.476668    -1.095359    -1.593654      85.38
 H      -0.057385    -1.844038    -2.335645      19.72
 C       2.516691    -0.027227    -0.867742      20.41
 C       4.095179     0.339966    -1.054472      88.50
 H       4.404224     0.170091    -2.027779      22.75
 O       4.333700     1.723759    -0.813643     276.52
 H       4.634164     1.958791     0.032031      27.35
 C       4.981049    -0.580439    -0.107407      79.05
 H       4.664734    -0.433500     0.881644      28.49
 O       4.681066    -2.007387    -0.327809     335.24
 H       5.054259    -2.315451    -1.157841      31.59
 C       6.637125    -0.470995    -0.299153     100.43
 O       7.119290     0.897654    -0.240276     258.49
 H       7.718946     1.117026     0.584947      28.10
 H       6.911297    -1.074004    -1.213059      32.48
 H       7.177710    -0.985633     0.513832      28.74
55
name= lig-ACN-Water-frame_162
 C      -4.331387     0.342953    -3.145996      39.54
 H      -4.623501    -0.602186    -3.664532      23.94
 C      -3.581257     1.584173    -1.197875      48.18
 H      -3.296981     1.717194    -0.145727      17.46
 C      -3.634792     2.734454    -2.044537      18.14
 O      -3.370089     4.096718    -1.723285     245.17
 C      -3.274833     4.244921    -0.210011     120.55
 H      -2.311070     3.781190     0.139310      25.30
 H      -4.187747     3.736428     0.116798      26.76
 H      -3.188738     5.242904    -0.014734      25.53
 C      -3.853985     2.658707    -3.437874       6.05
 O      -3.584938     3.732244    -4.343038      42.85
 H      -3.642022     4.558430    -3.792793      20.76
 C      -4.246318     1.408982    -3.974428      64.67
 H      -4.425574     1.286810    -4.986802      22.59
 C      -3.955173     0.368015    -1.790371      30.43
 C      -3.893603    -1.005700    -1.051585      55.59
 H      -4.630998    -1.650667    -1.481223      23.50
 O      -4.364835    -0.989351     0.370760      88.63
 H      -3.948663    -0.218039     0.879978      25.80
 C      -2.425860    -1.631404    -1.030302      83.84
 H      -2.276675    -1.855859    -2.190798      25.34
 C      -2.397071    -3.011802    -0.320440     120.56
 O      -3.077153    -4.083433    -1.056642     185.81
 H      -2.449564    -4.341859    -1.760346      28.56
 H      -2.649281    -2.770629     0.685677      25.92
 H      -1.277431    -3.287207    -0.225321      23.83
 C       1.879850    -0.910010    -1.768232      20.02
 H       2.251932    -1.464832    -2.625797      14.73
 C       1.860043     0.494820     0.291863      59.41
 H       2.332721     1.106431     0.911651      16.56
 C       0.480665     0.248524     0.469526      31.57
 O      -0.299469     0.982600     1.365728     218.96
 C       0.364963     1.622008     2.532223     104.04
 H      -0.565211     2.074725     3.067761      21.74
 H       0.943248     0.836848     3.184593      25.52
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 H       1.096153     2.281862     2.182623      26.61
 C      -0.210799    -0.480668    -0.533600      39.17
 O      -1.674376    -0.627286    -0.315075     152.65
 C       0.490907    -1.080899    -1.545938      65.29
 H      -0.062576    -1.787583    -2.327101      18.38
 C       2.622363    -0.051043    -0.883702      65.29
 C       4.086214     0.232000    -1.047672      89.38
 H       4.335405     0.029092    -2.049323      26.08
 O       4.202173     1.704841    -0.829698     183.95
 H       5.075943     1.835798    -0.296822      20.60
 C       5.049471    -0.654440    -0.120242      95.05
 H       4.887640    -0.357646     0.901522      25.46
 O       4.604774    -1.972540    -0.377120     323.74
 H       4.752062    -2.097318    -1.386520      26.73
 C       6.659485    -0.482576    -0.313233      99.93
 O       7.169891     0.894098    -0.269649     311.00
 H       7.200449     1.087458     0.737744      31.01
 H       6.934112    -0.712170    -1.328058      31.92
 H       7.090931    -1.193021     0.417511      29.71
55
name= lig-ACN-Water-frame_163
 C      -4.330399     0.286622    -3.125484      44.72
 H      -4.747202    -0.633439    -3.516830      25.81
 C      -3.638487     1.625167    -1.282641      57.06
 H      -3.382547     1.664165    -0.166205      18.83
 C      -3.560266     2.776043    -2.107251      19.97
 O      -3.421848     4.070815    -1.626799     246.26
 C      -3.334107     4.263422    -0.215042     125.22
 H      -2.505581     3.728073     0.241750      27.66
 H      -4.169473     3.973169     0.362332      27.60
 H      -3.297700     5.337953    -0.100319      25.01
 C      -3.750529     2.661663    -3.539840      13.69
 O      -3.588665     3.693063    -4.373363     158.59
 H      -3.208067     4.568895    -3.969320      20.20
 C      -4.261061     1.436037    -4.042713      63.80
 H      -4.431965     1.384720    -5.065284      16.65
 C      -3.997863     0.319639    -1.766336      37.42
 C      -3.863790    -1.002924    -1.017510      97.74
 H      -4.429638    -1.732544    -1.669734      24.13
 O      -4.378234    -1.042301     0.331762     137.32
 H      -3.927057    -0.226692     0.855424      22.99
 C      -2.481315    -1.630424    -1.072061      79.21
 H      -1.961381    -1.660125    -2.150913      22.75
 C      -2.389997    -3.001410    -0.277571     109.27
 O      -3.133138    -4.116698    -1.002042     146.60
 H      -2.543664    -4.389187    -1.819118      27.42
 H      -2.965804    -3.038653     0.590943      25.89
 H      -1.334866    -3.326118    -0.157065      24.69
 C       1.873758    -0.878894    -1.736433      28.36
 H       2.464102    -1.327034    -2.543145      19.58
 C       1.919948     0.509679     0.230668      77.42
 H       2.473925     1.074003     0.917986      19.52
 C       0.503760     0.324793     0.408509      21.66
 O      -0.308409     0.965766     1.340553     233.72
 C       0.294056     1.535494     2.481621     116.30
 H      -0.469471     2.231816     3.070354      22.86
 H       0.592027     0.643486     3.199527      23.26
 H       1.071794     2.274326     2.296438      24.85
 C      -0.259302    -0.498611    -0.501925      23.78
 O      -1.612134    -0.637073    -0.324865     176.19
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 C       0.488837    -1.116708    -1.568137      70.82
 H      -0.130382    -1.695219    -2.353701      18.12
 C       2.588338    -0.141898    -0.784334      46.54
 C       4.113169     0.199928    -1.033472      68.66
 H       4.356971    -0.039770    -2.055688      21.57
 O       4.148798     1.656473    -0.827194     219.16
 H       5.141718     1.998840    -0.781599      23.58
 C       5.100147    -0.607133    -0.162936      96.33
 H       4.837778    -0.570052     0.907538      23.24
 O       4.601147    -1.995671    -0.430419     334.11
 H       4.603800    -2.178795    -1.461568      24.14
 C       6.580082    -0.487972    -0.415600     104.96
 O       7.192268     0.856534    -0.237817     369.35
 H       6.975645     1.340843     0.545470      33.91
 H       6.787936    -0.864822    -1.360944      31.77
 H       7.150103    -1.153936     0.259886      27.45
55
name= lig-ACN-Water-frame_164
 C      -4.376143     0.242238    -3.216904      34.79
 H      -4.723380    -0.678032    -3.600835      22.84
 C      -3.676708     1.638419    -1.315487      59.15
 H      -3.476776     1.910749    -0.213213      17.86
 C      -3.529020     2.760632    -2.134725      24.44
 O      -3.451438     4.025299    -1.568137     219.42
 C      -3.393371     4.311233    -0.147092     123.80
 H      -2.545057     3.876422     0.325873      27.82
 H      -4.259107     4.055296     0.299857      29.03
 H      -3.155029     5.423925    -0.097110      24.71
 C      -3.690402     2.625849    -3.541656       9.84
 O      -3.569813     3.718108    -4.452538     123.26
 H      -3.367782     4.592001    -3.888045      19.66
 C      -4.199212     1.378636    -4.019845      66.59
 H      -4.564418     1.328383    -5.040392      24.05
 C      -3.999606     0.357544    -1.819075      32.09
 C      -3.884364    -1.021010    -1.050513      69.59
 H      -4.590912    -1.845406    -1.458796      23.09
 O      -4.408075    -1.012120     0.308346     156.88
 H      -3.792645    -0.524651     0.919135      25.22
 C      -2.395351    -1.607532    -1.011987      84.43
 H      -2.138387    -1.760424    -2.182901      24.55
 C      -2.428268    -3.028030    -0.314940     123.22
 O      -3.109596    -4.093984    -0.983961     186.55
 H      -2.598572    -4.376673    -1.796052      28.90
 H      -2.863413    -2.789381     0.634402      26.77
 H      -1.432617    -3.271522    -0.021996      27.39
 C       1.863903    -0.901767    -1.692693      25.34
 H       2.352291    -1.296318    -2.597569      17.30
 C       1.880393     0.504926     0.272612      90.11
 H       2.419557     1.248615     0.950803      16.60
 C       0.487149     0.396143     0.304609      26.60
 O      -0.338350     0.957631     1.288600     225.06
 C       0.262851     1.486563     2.532563      80.58
 H      -0.628364     2.136225     2.924159      22.59
 H       0.598606     0.648861     3.306241      22.51
 H       1.231383     2.022631     2.280434      21.72
 C      -0.193416    -0.567748    -0.536431      44.47
 O      -1.572658    -0.653791    -0.298320     196.77
 C       0.465940    -1.118713    -1.605975      64.42
 H       0.060128    -1.764252    -2.375449      19.52
 C       2.622580    -0.183458    -0.757918      42.08
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 C       4.061130     0.220682    -1.026589      92.07
 H       4.303116     0.015827    -2.082969      21.48
 O       4.166696     1.618694    -0.834351     275.58
 H       5.064962     1.838467    -0.665552      23.44
 C       4.985241    -0.659713    -0.180580      91.34
 H       4.852625    -0.321938     0.909620      22.87
 O       4.671197    -2.039730    -0.462399     361.63
 H       5.069303    -2.190099    -1.388063      26.64
 C       6.587503    -0.488272    -0.484803     103.17
 O       7.164718     0.815624    -0.290592     354.71
 H       6.997349     1.014748     0.677419      34.28
 H       6.775285    -0.660797    -1.472384      34.45
 H       7.016369    -1.271179     0.173998      29.50
55
name= lig-ACN-Water-frame_165
 C      -4.347433     0.240716    -3.220614      63.60
 H      -4.688659    -0.609332    -3.744294      25.72
 C      -3.691149     1.560735    -1.302514      64.58
 H      -3.606074     1.492691    -0.187519      22.74
 C      -3.566420     2.733936    -2.092106       6.50
 O      -3.440907     4.041068    -1.596420     191.72
 C      -3.413538     4.335243    -0.086598     109.96
 H      -2.678410     3.793759     0.404939      28.60
 H      -4.310142     4.181199     0.325585      27.73
 H      -3.296619     5.512512    -0.106395      24.41
 C      -3.700124     2.626983    -3.556743       2.19
 O      -3.546207     3.702754    -4.459120     107.11
 H      -3.634647     4.590963    -3.981226      20.02
 C      -4.128291     1.371524    -4.056424      55.60
 H      -4.343924     1.356746    -5.186634      22.47
 C      -4.006194     0.293016    -1.893079      30.73
 C      -3.883817    -0.980929    -1.057947      62.20
 H      -4.489873    -1.718651    -1.787766      22.65
 O      -4.437786    -0.930626     0.331157     143.31
 H      -3.788110    -0.501334     0.879122      26.73
 C      -2.404352    -1.615073    -1.021379      84.16
 H      -1.962090    -1.702763    -2.129312      25.88
 C      -2.375663    -2.961497    -0.257616     115.75
 O      -3.065630    -4.061270    -1.016022     179.87
 H      -2.435705    -4.291268    -1.686232      31.57
 H      -2.945737    -2.967968     0.693065      25.59
 H      -1.413602    -3.313942    -0.162545      27.27
 C       1.906189    -0.971277    -1.714191      54.09
 H       2.488823    -1.428424    -2.544797      16.13
 C       1.839651     0.490972     0.272005      62.68
 H       2.353993     1.306413     0.999963      12.92
 C       0.444454     0.351147     0.312111      32.38
 O      -0.357070     0.981299     1.265242     223.74
 C       0.242775     1.427639     2.533831      88.75
 H      -0.448869     2.165614     3.071244      24.03
 H       0.383963     0.463573     3.176262      22.85
 H       1.186882     2.146392     2.415031      21.12
 C      -0.190941    -0.538301    -0.572396      30.35
 O      -1.570087    -0.706668    -0.267799     189.60
 C       0.511337    -1.164741    -1.652779      61.35
 H      -0.023420    -1.765654    -2.277820      20.42
 C       2.539650    -0.106308    -0.770389      39.64
 C       3.989722     0.159793    -1.078863      72.58
 H       4.136535    -0.087327    -2.179987      21.83
 O       4.249645     1.636468    -0.812563     254.59
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 H       4.991638     1.749946    -0.201468      23.07
 C       5.019475    -0.688321    -0.221866      84.19
 H       4.743908    -0.658516     0.917896      24.89
 O       4.782479    -2.094579    -0.442774     367.49
 H       4.926677    -2.229543    -1.415559      29.12
 C       6.517704    -0.526359    -0.538845     104.05
 O       7.095389     0.798004    -0.312457     327.60
 H       7.596966     0.963964     0.573616      32.01
 H       6.620929    -0.729444    -1.548943      35.82
 H       7.133796    -1.294105    -0.044884      29.89
55
name= lig-ACN-Water-frame_166
 C      -4.261244     0.247097    -3.326600      34.62
 H      -4.616038    -0.717808    -3.661598      25.28
 C      -3.697181     1.498353    -1.300243      58.41
 H      -3.523665     1.666019    -0.260904      19.05
 C      -3.643644     2.716349    -2.058089      16.42
 O      -3.412616     4.052327    -1.571818     239.98
 C      -3.464660     4.318840    -0.160847     124.36
 H      -2.696730     3.816959     0.363171      27.62
 H      -4.342367     4.078700     0.276511      28.59
 H      -3.137290     5.463601    -0.012567      24.29
 C      -3.741972     2.648516    -3.492225      19.16
 O      -3.541131     3.650298    -4.393370     110.98
 H      -3.240330     4.494502    -3.991869      21.00
 C      -4.069148     1.412423    -4.117510      58.21
 H      -4.090070     1.319782    -5.289590      20.43
 C      -3.987606     0.256768    -1.879900      25.93
 C      -3.862612    -0.994652    -1.072290      72.37
 H      -4.561428    -1.946785    -1.355775      23.39
 O      -4.456422    -0.856894     0.279884     136.14
 H      -3.940207    -0.216765     0.910289      23.40
 C      -2.470278    -1.604734    -1.011464      86.07
 H      -2.093654    -1.766098    -2.098156      26.48
 C      -2.317737    -2.974791    -0.245860     120.93
 O      -3.002603    -4.004497    -1.054281     189.98
 H      -2.384793    -4.366378    -1.770852      26.01
 H      -2.779220    -2.929428     0.802816      25.83
 H      -1.329455    -3.078010    -0.025066      26.53
 C       1.916162    -0.998979    -1.726211      12.52
 H       2.604762    -1.546746    -2.407929      15.79
 C       1.784578     0.518771     0.216130      66.67
 H       2.483351     1.175817     0.975816      15.69
 C       0.422579     0.290952     0.407446      33.54
 O      -0.391485     1.040794     1.261702     239.62
 C       0.207843     1.371666     2.531917     113.40
 H      -0.602435     1.906055     3.023819      23.57
 H       0.525082     0.444799     3.130932      25.60
 H       1.268977     1.954856     2.367857      21.73
 C      -0.265303    -0.522555    -0.619750      32.07
 O      -1.565199    -0.734597    -0.249956     153.02
 C       0.503871    -1.220837    -1.612217      90.44
 H       0.093963    -1.825444    -2.313686      23.92
 C       2.489667    -0.089132    -0.867921      47.98
 C       4.037199     0.199888    -1.019580      75.44
 H       4.307864     0.102193    -2.150285      19.26
 O       4.337910     1.583489    -0.831064     264.25
 H       4.891551     1.873485     0.036971      21.91
 C       5.019149    -0.757157    -0.240006      93.43
 H       4.876087    -0.403664     0.900303      21.99
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 O       4.856238    -2.203089    -0.430123     335.87
 H       4.805357    -2.388532    -1.391533      26.59
 C       6.506433    -0.509448    -0.597880     102.98
 O       7.050014     0.808468    -0.344064     312.68
 H       7.625585     0.600223     0.384933      34.25
 H       6.582632    -0.682705    -1.649536      34.07
 H       7.031344    -1.292471    -0.043474      30.37
55
name= lig-ACN-Water-frame_167
 C      -4.145863     0.213788    -3.339956      58.02
 H      -4.343479    -0.646059    -4.010487      23.20
 C      -3.700749     1.571322    -1.294929      59.68
 H      -3.477939     1.581031    -0.286459      20.43
 C      -3.691825     2.737656    -2.047195      26.15
 O      -3.398554     3.986350    -1.598867     244.00
 C      -3.460194     4.264886    -0.175054     109.41
 H      -2.707021     3.699120     0.357829      26.26
 H      -4.427593     4.084722     0.151678      26.85
 H      -3.361820     5.441304    -0.135375      23.18
 C      -3.792863     2.600821    -3.462458      12.04
 O      -3.508155     3.658405    -4.305879      19.11
 H      -3.456764     4.535343    -3.849397      17.94
 C      -4.015696     1.383612    -4.083977      69.42
 H      -4.141873     1.495058    -5.236581      23.98
 C      -3.973145     0.286689    -1.968606      22.74
 C      -3.920664    -1.062034    -0.999598      54.77
 H      -4.557748    -1.833965    -1.723912      21.42
 O      -4.499837    -0.799946     0.248869     197.12
 H      -3.915651    -0.023101     0.715980      21.63
 C      -2.435562    -1.641490    -0.956212      93.43
 H      -2.178365    -1.730251    -2.060209      26.48
 C      -2.298191    -2.966557    -0.294154     130.18
 O      -2.946917    -3.981958    -1.049275     184.19
 H      -2.271393    -4.227720    -1.824382      25.56
 H      -2.860646    -2.915864     0.711088      24.63
 H      -1.329671    -3.313678    -0.218717      24.67
 C       1.846025    -1.009698    -1.717789      93.42
 H       2.237269    -1.591264    -2.575303      16.72
 C       1.786695     0.521302     0.134683      70.79
 H       2.277578     1.292363     0.894890      17.47
 C       0.400778     0.295295     0.327522      31.60
 O      -0.407956     1.031353     1.241254     231.73
 C       0.189237     1.321670     2.564993     117.13
 H      -0.488895     1.888482     3.155347      24.75
 H       0.477582     0.391577     3.071416      25.67
 H       1.054128     2.176974     2.409617      22.11
 C      -0.231514    -0.553411    -0.559007      37.71
 O      -1.632185    -0.705939    -0.269433     178.88
 C       0.468043    -1.252562    -1.562038      39.04
 H      -0.055193    -1.956500    -2.158439      17.20
 C       2.599626    -0.068414    -0.871063      87.69
 C       4.074296     0.184153    -1.007812      59.85
 H       4.296164    -0.115704    -2.134544      22.20
 O       4.403744     1.580263    -0.856743     247.55
 H       4.813476     1.896917     0.073221      23.02
 C       5.020248    -0.785844    -0.233406      86.20
 H       4.953374    -0.747593     0.961082      22.76
 O       4.849937    -2.262777    -0.386212     283.15
 H       5.230487    -2.383939    -1.321289      26.65
 C       6.516856    -0.515883    -0.687921     106.50
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 O       7.043670     0.808177    -0.363983     294.09
 H       7.533507     0.926983     0.468540      34.92
 H       6.708484    -0.690009    -1.781700      32.43
 H       7.130585    -1.254082    -0.181968      30.13
55
name= lig-ACN-Water-frame_168
 C      -4.032464     0.163916    -3.339770      45.07
 H      -4.195605    -0.908696    -3.663234      27.11
 C      -3.753924     1.501020    -1.318860      59.73
 H      -3.601560     1.606782    -0.270671      16.30
 C      -3.674039     2.684930    -2.082156      30.01
 O      -3.376618     3.969233    -1.626803     216.47
 C      -3.484831     4.222357    -0.177254     108.42
 H      -2.686237     3.725703     0.452569      26.48
 H      -4.425256     3.889373     0.302651      28.25
 H      -3.256474     5.319392    -0.076976      24.18
 C      -3.793273     2.633534    -3.473894      12.47
 O      -3.487740     3.698618    -4.243826      11.47
 H      -3.585674     4.612810    -3.811407      14.94
 C      -4.003523     1.375494    -4.096720      66.26
 H      -4.135651     1.306803    -5.207844      22.90
 C      -3.909359     0.248348    -1.899002      38.75
 C      -3.921968    -0.971460    -1.111629      59.73
 H      -4.664455    -1.911881    -1.463788      21.33
 O      -4.579858    -0.788614     0.242611     144.55
 H      -3.872343    -0.317753     0.885542      20.49
 C      -2.459101    -1.610180    -1.013367      80.11
 H      -2.020831    -1.704241    -2.009573      25.46
 C      -2.270262    -3.020787    -0.273159     114.31
 O      -2.974962    -4.032997    -1.068413     225.44
 H      -2.384905    -4.333085    -1.865114      26.51
 H      -2.706475    -3.051942     0.789757      24.16
 H      -1.210130    -3.101006    -0.059988      25.81
 C       1.832660    -0.990426    -1.707874     -11.60
 H       2.465500    -1.418646    -2.500795      16.35
 C       1.825381     0.581142     0.112990     100.28
 H       2.296536     1.418705     0.673740      14.91
 C       0.439611     0.406477     0.246349      31.76
 O      -0.379026     0.985700     1.232503     238.45
 C       0.170522     1.328117     2.561093      88.25
 H      -0.681419     1.659755     3.067014      24.57
 H       0.586679     0.465665     3.021901      24.71
 H       1.120074     2.077969     2.536156      20.72
 C      -0.321611    -0.646925    -0.460533      39.76
 O      -1.650374    -0.611068    -0.280096     189.85
 C       0.426434    -1.261540    -1.486073      79.68
 H      -0.027473    -2.034606    -2.183658      19.07
 C       2.524758    -0.164335    -0.864015      47.87
 C       4.093641     0.086513    -1.050347      52.38
 H       4.369582    -0.064063    -2.212025      19.45
 O       4.424778     1.579240    -0.922236     250.95
 H       4.787897     1.811773    -0.068314      25.00
 C       5.136291    -0.844828    -0.207440      81.26
 H       4.934157    -0.510539     0.927313      22.30
 O       4.827099    -2.242524    -0.378666     330.07
 H       4.986457    -2.595091    -1.344886      26.37
 C       6.579743    -0.531131    -0.661068      92.04
 O       7.056548     0.834442    -0.407789     317.30
 H       7.206878     0.694598     0.599142      33.03
 H       6.416230    -0.535199    -1.809868      31.17
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 H       7.277170    -1.300752    -0.347638      28.80
55
name= lig-ACN-Water-frame_169
 C      -3.950488     0.170994    -3.285634      61.76
 H      -4.143137    -0.764985    -3.872710      19.73
 C      -3.789667     1.503191    -1.284514      65.26
 H      -3.838905     1.582249    -0.166803      18.29
 C      -3.628424     2.636621    -2.073726       5.06
 O      -3.375135     3.946854    -1.583949     218.82
 C      -3.458962     4.175658    -0.167638     107.27
 H      -2.563159     3.601111     0.306208      24.53
 H      -4.498554     3.836425     0.177794      26.26
 H      -3.447616     5.233108    -0.015130      23.97
 C      -3.749536     2.577920    -3.535257      -3.85
 O      -3.500883     3.745379    -4.279804     121.81
 H      -3.202202     4.535141    -3.713276      19.17
 C      -3.996184     1.301945    -4.123595      61.50
 H      -4.037289     1.263634    -5.178649      24.60
 C      -3.886142     0.258318    -1.931403      34.04
 C      -3.899017    -1.026413    -1.044776      66.51
 H      -4.515550    -1.833864    -1.793216      22.15
 O      -4.605884    -0.825668     0.212166     172.01
 H      -3.957044    -0.354966     0.813388      23.46
 C      -2.481051    -1.581581    -0.994059      91.98
 H      -2.243888    -1.709857    -2.027245      26.14
 C      -2.309913    -3.012243    -0.279558     113.72
 O      -3.013764    -4.084610    -1.036349     201.84
 H      -2.384596    -4.431871    -1.687218      29.66
 H      -2.803309    -2.953331     0.719455      23.87
 H      -1.234532    -3.370610    -0.305050      22.44
 C       1.788110    -1.047467    -1.688225      77.90
 H       2.183076    -1.654351    -2.511542      22.91
 C       1.826612     0.662873     0.100911      67.88
 H       2.376877     1.346566     0.638302      20.76
 C       0.433538     0.406549     0.286700       4.48
 O      -0.328471     0.997280     1.246639     249.11
 C       0.177032     1.311451     2.534783     109.27
 H      -0.654273     1.692996     3.084207      23.79
 H       0.605497     0.505848     3.037347      25.10
 H       0.821248     2.284189     2.446219      21.95
 C      -0.227506    -0.582348    -0.473748      12.86
 O      -1.700059    -0.573724    -0.297705     179.66
 C       0.442119    -1.312165    -1.474578      58.20
 H      -0.134290    -2.017400    -2.235472      18.03
 C       2.580351    -0.155893    -0.814294      58.92
 C       4.101317     0.070253    -1.067452      65.79
 H       4.269018    -0.276322    -2.223515      21.79
 O       4.376650     1.477486    -1.033746     278.02
 H       4.777579     1.791308    -0.235390      26.03
 C       5.144814    -0.810811    -0.228260      89.84
 H       5.097852    -0.636677     0.940528      22.07
 O       4.806119    -2.222129    -0.360795     326.70
 H       4.730337    -2.255379    -1.356081      25.08
 C       6.614036    -0.520426    -0.721895      93.45
 O       7.084093     0.797824    -0.372545     326.72
 H       7.324524     0.998574     0.543519      33.86
 H       6.711578    -0.595184    -1.923943      30.55
 H       7.316916    -1.279819    -0.364704      28.36
55
name= lig-ACN-Water-frame_170
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 C      -3.957726     0.159725    -3.336222      39.41
 H      -4.124652    -0.868407    -3.703517      30.51
 C      -3.810760     1.540506    -1.267908      51.39
 H      -3.865536     1.633265    -0.122087      21.55
 C      -3.595097     2.673970    -2.099075      15.12
 O      -3.390864     3.901902    -1.593122     174.77
 C      -3.442558     4.112457    -0.150223     109.38
 H      -2.592671     3.642476     0.529067      25.95
 H      -4.442283     3.691632     0.364298      23.86
 H      -3.342178     5.122304    -0.044710      25.72
 C      -3.633562     2.578140    -3.530029      18.54
 O      -3.531279     3.666090    -4.336637      85.91
 H      -3.511730     4.572806    -3.790884      18.38
 C      -3.911440     1.341416    -4.155626      89.53
 H      -4.069598     1.254845    -5.159155      27.48
 C      -3.900027     0.235702    -1.869713     -55.28
 C      -3.909862    -1.061112    -1.042254      50.11
 H      -4.546996    -2.016380    -1.549246      21.75
 O      -4.608495    -0.910351     0.186404     160.00
 H      -4.079265    -0.338140     0.737272      27.22
 C      -2.458505    -1.629838    -0.951697      97.93
 H      -2.128778    -1.676788    -1.940936      30.16
 C      -2.382566    -3.003942    -0.328645     130.04
 O      -3.069554    -4.100067    -0.965368     207.34
 H      -2.453060    -4.404610    -1.654930      29.71
 H      -2.723614    -2.988045     0.704459      26.89
 H      -1.221860    -3.201653    -0.121894      24.29
 C       1.857127    -1.129464    -1.606080      18.85
 H       2.456758    -1.649098    -2.349653      19.54
 C       1.854573     0.637784     0.088567      59.58
 H       2.202307     1.313731     0.708569      20.97
 C       0.495202     0.347267     0.351646      34.57
 O      -0.361369     1.040090     1.249967     236.45
 C       0.209203     1.400020     2.571753     109.72
 H      -0.658571     1.628988     3.209232      24.28
 H       0.748583     0.578077     2.952316      27.11
 H       0.950162     2.239990     2.507488      24.93
 C      -0.273560    -0.493471    -0.556850      23.20
 O      -1.618003    -0.590928    -0.336205     187.65
 C       0.430396    -1.289940    -1.459268      73.40
 H      -0.194841    -2.044677    -2.148324      22.00
 C       2.554031    -0.164921    -0.844101      37.15
 C       4.056637     0.016642    -1.059107      84.67
 H       4.257780    -0.417665    -2.166916      23.24
 O       4.343359     1.426497    -1.174883     247.38
 H       4.892536     1.723197    -0.316438      22.13
 C       5.129519    -0.758128    -0.285325      89.73
 H       5.108492    -0.486532     0.843085      24.21
 O       4.785283    -2.169421    -0.377257     280.89
 H       4.910669    -2.531140    -1.265533      30.20
 C       6.636668    -0.524964    -0.730598      86.50
 O       7.136835     0.806112    -0.353839     277.40
 H       7.500599     0.596778     0.505410      32.11
 H       6.769375    -0.590234    -1.939257      30.52
 H       7.177151    -1.343807    -0.211140      29.79
55
name= lig-ACN-Water-frame_171
 C      -3.996697     0.165949    -3.284215      69.00
 H      -4.158100    -0.758888    -3.803005      25.86
 C      -3.806751     1.489839    -1.331874      68.28
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 H      -3.750134     1.694994    -0.228104      19.64
 C      -3.582643     2.622191    -2.084293      10.00
 O      -3.391301     3.937253    -1.569170     199.62
 C      -3.421144     4.083196    -0.115153     103.87
 H      -2.481066     3.487765     0.257433      24.55
 H      -4.504924     3.726819     0.347171      25.35
 H      -3.347993     5.105858     0.059077      25.57
 C      -3.581342     2.557927    -3.522698       3.40
 O      -3.552634     3.635414    -4.396547     106.98
 H      -3.576673     4.575222    -3.971452      20.43
 C      -3.803558     1.301740    -4.107589      56.50
 H      -3.961810     1.383678    -5.126815      23.91
 C      -3.958988     0.238474    -1.913621      38.09
 C      -3.886676    -1.050186    -1.105766      51.12
 H      -4.430815    -1.939269    -1.746755      21.54
 O      -4.617796    -0.986159     0.223735     133.87
 H      -4.045921    -0.630227     0.987943      22.61
 C      -2.433438    -1.622801    -1.041437      87.04
 H      -2.131382    -1.831293    -2.014772      29.42
 C      -2.363135    -3.020193    -0.183653     104.98
 O      -3.087854    -4.088054    -0.944487     144.95
 H      -2.540174    -4.393550    -1.762643      28.28
 H      -2.885074    -2.907224     0.725380      25.87
 H      -1.195150    -3.368793    -0.127772      22.53
 C       1.879810    -1.211346    -1.543283      69.67
 H       2.410010    -1.893758    -2.193358      15.29
 C       1.827374     0.562065     0.172501      50.89
 H       2.453010     1.251628     0.553364      14.95
 C       0.426042     0.375855     0.344368      23.72
 O      -0.344919     1.082768     1.262496     223.03
 C       0.272405     1.456555     2.586135     102.93
 H      -0.606309     1.716866     3.246337      23.46
 H       0.831936     0.600203     3.003011      26.09
 H       0.866065     2.313038     2.495644      24.81
 C      -0.224967    -0.491060    -0.583969      37.95
 O      -1.614044    -0.632815    -0.321942     183.03
 C       0.507156    -1.257527    -1.495238      69.98
 H       0.041824    -2.100927    -2.142066      18.13
 C       2.546153    -0.193410    -0.818898      65.79
 C       4.027030    -0.003951    -1.191759      69.35
 H       4.123579    -0.353437    -2.324829      19.62
 O       4.367740     1.441107    -1.292848     265.86
 H       4.958563     1.793072    -0.514465      22.30
 C       5.108565    -0.735603    -0.307893      90.62
 H       4.973235    -0.411851     0.757229      24.90
 O       4.799691    -2.146432    -0.371482     329.90
 H       4.954121    -2.316782    -1.328317      28.33
 C       6.590066    -0.506511    -0.699628      86.30
 O       7.204912     0.758345    -0.349690     305.18
 H       7.590902     0.906937     0.597612      30.34
 H       6.650392    -0.672749    -1.910726      31.10
 H       7.228745    -1.334967    -0.279316      29.35
55
name= lig-ACN-Water-frame_172
 C      -4.041276     0.123178    -3.346061      68.79
 H      -4.273932    -0.782923    -3.843055      29.91
 C      -3.755119     1.486124    -1.298712      53.55
 H      -3.739391     1.374667    -0.233117      20.31
 C      -3.561856     2.701488    -2.095278      21.00
 O      -3.420392     3.948957    -1.556082     190.73
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 C      -3.371463     4.062672    -0.116777      90.36
 H      -2.576489     3.441146     0.445657      25.89
 H      -4.423595     3.603034     0.396969      24.46
 H      -3.196920     5.109767     0.141841      25.21
 C      -3.604003     2.576446    -3.521893      19.41
 O      -3.556787     3.641141    -4.421630     144.06
 H      -3.252356     4.396773    -3.916150      24.08
 C      -3.730079     1.282004    -4.082229      49.33
 H      -3.692093     1.088472    -5.150542      22.18
 C      -4.006359     0.205293    -1.916429       3.33
 C      -3.885885    -1.080371    -1.106981      70.59
 H      -4.452119    -1.885597    -1.731426      22.65
 O      -4.564534    -1.059100     0.204722     172.31
 H      -3.830664    -0.530894     0.782179      22.44
 C      -2.401274    -1.677948    -1.003736      91.79
 H      -2.044123    -1.754781    -1.991609      27.92
 C      -2.372707    -3.002762    -0.177863     113.63
 O      -3.060305    -4.051770    -0.926765     183.02
 H      -2.348966    -4.252916    -1.621563      28.02
 H      -2.841161    -2.874775     0.777028      26.14
 H      -1.262211    -3.401896     0.198874      23.23
 C       1.928278    -1.255550    -1.528456      50.95
 H       2.443480    -1.948131    -2.189855      16.82
 C       1.868872     0.494246     0.191562      70.41
 H       2.180583     1.267519     0.869850      14.48
 C       0.432633     0.451309     0.305063      19.04
 O      -0.318565     1.113083     1.303600     241.24
 C       0.323941     1.476706     2.533796     100.08
 H      -0.532527     1.853861     3.201224      24.27
 H       0.855892     0.598133     3.032319      23.78
 H       0.941018     2.263009     2.394632      24.76
 C      -0.218680    -0.533848    -0.527788      19.26
 O      -1.633491    -0.672432    -0.340662     189.56
 C       0.496406    -1.309752    -1.510620      62.26
 H      -0.085730    -1.993650    -2.133673      19.10
 C       2.596513    -0.255781    -0.762756      27.82
 C       4.055062     0.090382    -1.280779      62.59
 H       4.125826    -0.384824    -2.324237      20.01
 O       4.412393     1.466429    -1.402996     303.32
 H       4.930365     1.641730    -0.658446      23.69
 C       5.033917    -0.687767    -0.308923      85.07
 H       4.799534    -0.422407     0.724853      23.22
 O       4.849120    -2.141333    -0.382637     296.50
 H       4.667543    -2.458532    -1.335685      25.83
 C       6.579231    -0.495730    -0.651251      73.08
 O       7.273579     0.739548    -0.386071     302.49
 H       7.096589     0.907912     0.585757      32.76
 H       6.677216    -0.467544    -1.846735      28.54
 H       7.080374    -1.436756    -0.225112      27.72
55
name= lig-ACN-Water-frame_173
 C      -4.052897     0.106261    -3.335649      64.46
 H      -4.253511    -0.846147    -3.770788      28.05
 C      -3.704707     1.482268    -1.319656      69.58
 H      -3.586942     1.724167    -0.327321      20.32
 C      -3.602304     2.647840    -2.068649       8.04
 O      -3.431831     3.968520    -1.546046     192.76
 C      -3.330518     4.026356    -0.071279      88.20
 H      -2.475040     3.412928     0.254871      25.70
 H      -4.465047     3.808735     0.447369      24.23
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 H      -3.126409     5.161135     0.098351      23.37
 C      -3.626178     2.567009    -3.522590      -4.68
 O      -3.517170     3.660827    -4.380119     153.45
 H      -3.369132     4.554461    -4.023178      22.44
 C      -3.731933     1.259465    -4.133927      41.45
 H      -3.594932     1.390674    -5.265870      20.03
 C      -3.970370     0.194161    -1.925385      29.37
 C      -3.890284    -1.171907    -1.119380      93.42
 H      -4.391294    -2.069656    -1.582859      24.63
 O      -4.436901    -1.066751     0.164974     142.01
 H      -4.073452    -0.347712     0.805873      22.42
 C      -2.402990    -1.692748    -0.967973      88.49
 H      -2.053834    -1.994922    -1.941779      28.48
 C      -2.391571    -2.975033    -0.167453     116.17
 O      -2.988880    -4.036126    -0.930008     206.63
 H      -2.451710    -4.438005    -1.598948      29.99
 H      -3.016165    -2.856202     0.739218      25.28
 H      -1.209407    -3.147562     0.043141      23.74
 C       1.901154    -1.229374    -1.530016      24.91
 H       2.461731    -1.677312    -2.358341      16.03
 C       1.872202     0.513903     0.198490     102.24
 H       2.632019     1.128985     0.808998      20.16
 C       0.488334     0.382169     0.298967      19.58
 O      -0.297247     1.085807     1.252826     232.25
 C       0.395794     1.515449     2.500589      96.34
 H      -0.425673     1.912519     3.178268      23.29
 H       0.872987     0.564049     2.980236      24.39
 H       1.148508     2.171661     2.347004      26.21
 C      -0.256687    -0.584452    -0.506659      23.83
 O      -1.597625    -0.648165    -0.317676     185.71
 C       0.472587    -1.358574    -1.399600      57.22
 H       0.038373    -2.001291    -2.070968      22.50
 C       2.625696    -0.266637    -0.797393      79.06
 C       4.067104     0.053329    -1.228231      73.82
 H       4.185006    -0.290562    -2.278861      23.51
 O       4.464858     1.495389    -1.480120     270.60
 H       4.916765     1.944667    -0.724373      27.04
 C       5.061725    -0.660419    -0.355030     105.46
 H       4.851304    -0.342845     0.637547      25.97
 O       4.851240    -2.114605    -0.377002     240.46
 H       4.956434    -2.365460    -1.400725      28.09
 C       6.552179    -0.495742    -0.675386      88.93
 O       7.295861     0.743204    -0.378895     296.86
 H       7.222251     1.092451     0.499798      33.32
 H       6.661949    -0.861152    -1.791671      30.31
 H       7.106237    -1.285778    -0.030024      28.69
55
name= lig-ACN-Water-frame_174
 C      -3.989257     0.168271    -3.341536      45.58
 H      -4.126958    -0.765928    -3.899628      30.08
 C      -3.683705     1.430451    -1.322322      50.16
 H      -3.539471     1.340942    -0.303402      22.61
 C      -3.644360     2.653454    -2.111685      11.82
 O      -3.461820     3.902976    -1.532870     200.86
 C      -3.291242     4.051353    -0.090484      79.36
 H      -2.541539     3.402263     0.327406      28.46
 H      -4.284537     3.669000     0.564513      22.46
 H      -2.944178     5.190002     0.169845      23.03
 C      -3.630895     2.548589    -3.528037      18.09
 O      -3.466442     3.677752    -4.322856      67.45
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 H      -3.636271     4.419062    -3.636768      23.94
 C      -3.801035     1.314094    -4.135736      51.99
 H      -3.955867     1.131388    -5.284988      19.42
 C      -3.882656     0.167835    -1.930145       5.47
 C      -3.800157    -1.126467    -1.164658      73.31
 H      -4.374420    -1.807606    -1.761642      22.82
 O      -4.416511    -1.049950     0.197954     143.41
 H      -3.817813    -0.448021     0.625582      28.18
 C      -2.399205    -1.664569    -1.014747      87.02
 H      -1.930162    -1.740468    -2.028520      26.60
 C      -2.346300    -2.972933    -0.132856     107.21
 O      -2.960337    -4.085120    -0.944808     196.86
 H      -2.234249    -4.200715    -1.604369      28.75
 H      -2.917473    -2.949556     0.858835      24.15
 H      -1.271115    -3.351313     0.211901      22.90
 C       1.849129    -1.135885    -1.591709      78.41
 H       2.213795    -1.750519    -2.429559      20.61
 C       1.948570     0.488397     0.146148      48.99
 H       2.384387     1.376793     0.830093      15.21
 C       0.527227     0.293971     0.378613      34.63
 O      -0.245470     1.051312     1.201867     235.36
 C       0.463688     1.490563     2.436715     109.05
 H      -0.291167     2.067449     3.009836      24.80
 H       0.844041     0.564537     3.041893      25.39
 H       1.168744     2.218818     2.166719      26.17
 C      -0.183850    -0.588265    -0.457308      19.08
 O      -1.630893    -0.620344    -0.282737     163.86
 C       0.532066    -1.457084    -1.339657      58.28
 H       0.040421    -2.163045    -1.864538      19.94
 C       2.576770    -0.176766    -0.857936      47.19
 C       4.077524     0.054930    -1.245127      68.74
 H       4.155583    -0.429395    -2.175631      24.10
 O       4.480762     1.492956    -1.509018     251.16
 H       4.741848     1.813381    -0.523267      24.11
 C       5.142649    -0.660151    -0.305702     101.17
 H       5.066308    -0.414119     0.710971      25.70
 O       4.829473    -2.062478    -0.379503     283.66
 H       4.991979    -2.433941    -1.308317      26.71
 C       6.646582    -0.515643    -0.625508      93.53
 O       7.273435     0.767520    -0.459849     310.94
 H       7.550177     0.833030     0.501006      30.08
 H       6.928074    -0.668155    -1.702801      30.57
 H       7.080572    -1.387881     0.025316      28.50
55
name= lig-ACN-Water-frame_175
 C      -3.908973     0.150115    -3.382840      68.97
 H      -4.137526    -0.847307    -3.837850      20.60
 C      -3.676930     1.419980    -1.324399      72.71
 H      -3.609304     1.586455    -0.251788      20.75
 C      -3.629691     2.569728    -2.048955       7.42
 O      -3.499079     3.855671    -1.533992     209.29
 C      -3.241369     4.006137    -0.104433      99.18
 H      -2.408984     3.442536     0.236040      26.53
 H      -4.317309     3.899011     0.473314      22.40
 H      -3.020528     5.231602    -0.073098      22.28
 C      -3.654182     2.582863    -3.507460       0.66
 O      -3.441211     3.724597    -4.230830      45.46
 H      -3.373570     4.694850    -3.823641      18.36
 C      -3.923172     1.334457    -4.142023      55.97
 H      -4.123415     1.364410    -5.294854      25.54
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 C      -3.774614     0.208148    -1.996068      44.80
 C      -3.788980    -1.077156    -1.156173      86.56
 H      -4.298318    -1.851830    -1.592873      27.91
 O      -4.411754    -1.006871     0.166187     186.18
 H      -3.930840    -0.760892     0.943469      23.78
 C      -2.285414    -1.650863    -0.974331      77.73
 H      -1.862765    -1.864326    -2.030155      24.00
 C      -2.308521    -3.049674    -0.191158     108.79
 O      -2.902822    -4.107008    -0.925260     230.13
 H      -2.468790    -4.318209    -1.856428      27.69
 H      -2.998561    -2.769745     0.701137      23.74
 H      -1.222006    -3.200473     0.113341      24.54
 C       1.883675    -1.108454    -1.700079      51.38
 H       2.560107    -1.693451    -2.349378      16.51
 C       1.911616     0.522151     0.160428      63.65
 H       2.473517     1.449553     0.687180      16.64
 C       0.579708     0.235230     0.376687      14.00
 O      -0.193918     1.037918     1.246872     252.61
 C       0.477470     1.500672     2.369869     113.04
 H      -0.269114     1.981371     2.997607      24.09
 H       0.923373     0.621039     2.975876      24.73
 H       1.405917     2.075594     2.171548      24.08
 C      -0.214972    -0.688912    -0.385484       9.54
 O      -1.572770    -0.606545    -0.258352     202.01
 C       0.492133    -1.480052    -1.287780      94.52
 H       0.083504    -2.312510    -1.800067      22.17
 C       2.625618    -0.116190    -0.981800      43.80
 C       4.139782     0.093135    -1.289796      91.40
 H       4.347189    -0.284651    -2.225534      24.45
 O       4.450252     1.440893    -1.468005     272.75
 H       4.736449     1.925103    -0.646201      26.20
 C       5.161276    -0.658581    -0.265138      92.33
 H       4.911443    -0.324248     0.687991      26.90
 O       4.809393    -2.068565    -0.356679     319.33
 H       4.678295    -2.252214    -1.291956      28.48
 C       6.768357    -0.546718    -0.636443      92.76
 O       7.261112     0.801341    -0.521991     293.07
 H       7.754747     1.023960     0.361396      27.59
 H       6.707696    -0.928923    -1.652232      32.75
 H       7.448484    -1.248384    -0.010652      27.62
55
name= lig-ACN-Water-frame_176
 C      -3.888864     0.147413    -3.428304       9.80
 H      -4.105592    -0.825477    -3.963074      17.21
 C      -3.663634     1.425086    -1.286063      60.87
 H      -3.769451     1.372188    -0.146281      20.65
 C      -3.584216     2.616323    -2.063721      21.78
 O      -3.522625     3.837714    -1.529189     233.86
 C      -3.242530     4.028248    -0.150338      98.45
 H      -2.413951     3.415909     0.191181      28.42
 H      -4.084362     3.705011     0.601791      24.02
 H      -2.897900     5.212581     0.022150      23.19
 C      -3.703978     2.594126    -3.453618       8.60
 O      -3.430778     3.762613    -4.207922     115.28
 H      -3.461345     4.525289    -3.551363      18.19
 C      -3.992296     1.412463    -4.156343      54.12
 H      -4.083848     1.512278    -5.275553      26.43
 C      -3.715952     0.160382    -1.969314     -13.94
 C      -3.679648    -1.139188    -1.099343      97.64
 H      -4.174865    -1.810782    -1.640278      28.13
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 O      -4.462088    -0.957536     0.133089     180.03
 H      -3.768076    -0.426802     0.661240      25.90
 C      -2.302697    -1.673679    -0.949847      94.66
 H      -1.815477    -1.692776    -2.036461      24.32
 C      -2.246373    -3.006455    -0.242402     127.25
 O      -2.881539    -4.158769    -0.927044     208.31
 H      -2.346602    -4.235187    -1.793359      29.13
 H      -2.848662    -3.069855     0.727719      24.30
 H      -1.269284    -3.363257     0.102866      27.40
 C       1.888237    -1.127334    -1.663914      28.62
 H       2.189793    -1.726969    -2.535911      18.73
 C       1.966616     0.519553     0.014154      76.38
 H       2.551884     1.253861     0.694627      19.86
 C       0.565307     0.273355     0.359217      34.57
 O      -0.185870     0.998479     1.250338     217.54
 C       0.555354     1.505019     2.462440     105.19
 H      -0.133349     2.094120     3.032084      25.52
 H       0.920757     0.601918     3.011506      25.02
 H       1.283785     2.345675     2.130682      23.70
 C      -0.107140    -0.755476    -0.340178      35.09
 O      -1.507472    -0.675511    -0.226319     164.96
 C       0.621596    -1.468289    -1.366359      81.11
 H       0.077936    -2.282452    -1.938578      17.13
 C       2.629409    -0.122448    -1.002217      55.56
 C       4.215614     0.059100    -1.309145      78.85
 H       4.363294    -0.376831    -2.211203      29.44
 O       4.442521     1.535269    -1.426814     253.96
 H       4.772226     1.779567    -0.602689      28.26
 C       5.168373    -0.675434    -0.293777      96.98
 H       5.046792    -0.357708     0.697170      26.91
 O       4.794607    -2.089025    -0.318209     293.28
 H       4.620347    -2.348925    -1.242734      28.85
 C       6.710576    -0.546725    -0.634950     102.94
 O       7.269631     0.846417    -0.653545     273.32
 H       7.444719     0.979237     0.332382      29.45
 H       6.971897    -0.811265    -1.604733      31.62
 H       7.255652    -1.221235     0.093829      29.03
55
name= lig-ACN-Water-frame_177
 C      -3.920267     0.234166    -3.362316      88.67
 H      -3.980081    -0.684632    -3.972647      29.27
 C      -3.649144     1.369503    -1.330079      58.03
 H      -3.613874     1.498985    -0.176698      20.21
 C      -3.601373     2.580323    -2.021381     -14.49
 O      -3.541561     3.944539    -1.517159     188.96
 C      -3.206075     4.021997    -0.100346     121.00
 H      -2.283855     3.424593     0.163341      25.02
 H      -4.129159     3.721434     0.462290      26.70
 H      -3.056715     5.205042     0.091385      23.91
 C      -3.712809     2.620615    -3.484839       1.23
 O      -3.464141     3.719562    -4.186732      27.83
 H      -3.567505     4.640146    -3.887422      14.58
 C      -3.964995     1.400447    -4.113073      76.48
 H      -4.135213     1.295319    -5.155758      24.32
 C      -3.717134     0.140938    -2.013247      27.13
 C      -3.718929    -1.136052    -1.173119      67.86
 H      -4.155738    -1.919826    -1.576288      27.85
 O      -4.459070    -0.919895     0.098296     112.63
 H      -4.113139    -0.313634     0.860303      23.11
 C      -2.244617    -1.703504    -0.938555      71.81
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 H      -1.905360    -1.897590    -2.082136      24.69
 C      -2.198042    -3.104147    -0.172477     116.27
 O      -2.845719    -4.177777    -0.977725     206.64
 H      -2.330576    -4.361501    -1.756174      30.17
 H      -2.632728    -2.851024     0.823503      26.03
 H      -1.168625    -3.218467    -0.101723      27.97
 C       2.019925    -1.197028    -1.735254      28.29
 H       2.540957    -1.584348    -2.619503      17.04
 C       1.982980     0.557936    -0.012937      71.53
 H       2.502523     1.316679     0.556760      18.49
 C       0.658119     0.309703     0.316284      22.39
 O      -0.151170     0.993076     1.317311     218.07
 C       0.572113     1.512607     2.506368     103.79
 H      -0.221910     1.916092     3.111294      24.61
 H       1.123484     0.776804     3.082528      26.62
 H       1.485821     2.223634     2.144188      22.57
 C      -0.028294    -0.739421    -0.392373      30.69
 O      -1.424889    -0.805503    -0.161440     173.92
 C       0.584842    -1.456868    -1.376568      94.43
 H       0.052081    -2.154048    -2.164915      20.72
 C       2.722322    -0.229964    -1.020141      54.77
 C       4.147471     0.098451    -1.317875      85.73
 H       4.403050    -0.182014    -2.265351      25.06
 O       4.466814     1.583139    -1.386128     233.89
 H       4.725950     1.973473    -0.503797      25.64
 C       5.155501    -0.671856    -0.373855     102.07
 H       4.979906    -0.337789     0.614509      27.44
 O       4.807586    -2.091891    -0.290354     227.33
 H       4.853701    -2.498825    -1.243183      31.88
 C       6.646907    -0.499635    -0.684093     110.88
 O       7.240362     0.830318    -0.736637     272.21
 H       7.383474     1.235610     0.102962      32.28
 H       6.766591    -1.021476    -1.570627      33.89
 H       7.149683    -1.064684     0.119260      29.85
55
name= lig-ACN-Water-frame_178
 C      -3.965664     0.158471    -3.389824      53.26
 H      -4.085295    -0.791501    -3.873778      28.65
 C      -3.604740     1.434635    -1.320839      52.19
 H      -3.339849     1.391334    -0.222294      21.12
 C      -3.661425     2.670225    -2.026623      18.48
 O      -3.536408     3.952355    -1.493057     220.28
 C      -3.237070     4.031455    -0.043325     110.10
 H      -2.247040     3.483180     0.217213      26.45
 H      -3.972088     3.628657     0.584366      27.02
 H      -3.061802     5.158288     0.199707      24.32
 C      -3.706472     2.620573    -3.421993      -0.53
 O      -3.516803     3.724246    -4.288404      89.18
 H      -3.439434     4.505664    -3.736099      22.63
 C      -3.912007     1.383386    -4.110031      61.03
 H      -4.036241     1.487607    -5.127238      20.71
 C      -3.761394     0.182187    -1.954962       0.32
 C      -3.715485    -1.124756    -1.154346      74.44
 H      -4.248683    -1.762711    -1.689524      26.91
 O      -4.487625    -0.946738     0.064515     185.73
 H      -3.862844    -0.378211     0.529500      30.64
 C      -2.235844    -1.797066    -0.920946      75.73
 H      -1.646744    -1.900312    -1.967059      23.93
 C      -2.147333    -3.152009    -0.201640     126.22
 O      -2.799080    -4.172316    -0.964205     203.84
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 H      -2.359698    -4.177434    -1.845278      30.08
 H      -2.739360    -3.325486     0.690876      25.66
 H      -1.207072    -3.434897     0.095798      27.65
 C       2.050929    -1.242854    -1.774863      39.46
 H       2.546432    -1.902105    -2.486572      21.78
 C       2.064130     0.567155    -0.005508      50.70
 H       2.541380     1.419419     0.263157      16.96
 C       0.675915     0.315026     0.341033      15.57
 O      -0.028968     0.945986     1.343994     208.41
 C       0.603043     1.480339     2.503617     109.09
 H      -0.156465     1.963779     3.138080      24.49
 H       1.033239     0.652336     2.980983      26.10
 H       1.271054     2.503364     2.287952      22.29
 C      -0.035961    -0.663806    -0.477299       9.38
 O      -1.347413    -0.920871    -0.089457     179.35
 C       0.718068    -1.443425    -1.501583      58.60
 H      -0.005530    -2.163786    -2.074455      20.01
 C       2.700977    -0.223289    -0.970218      39.88
 C       4.168917     0.193226    -1.384892      84.83
 H       4.239478    -0.130386    -2.376892      25.46
 O       4.453235     1.569850    -1.361574     285.68
 H       4.745302     1.801524    -0.383340      22.95
 C       5.068217    -0.601317    -0.382433     103.47
 H       4.809789    -0.243181     0.602619      26.06
 O       4.858410    -2.068340    -0.311879     267.48
 H       4.934346    -2.416992    -1.257206      29.36
 C       6.641338    -0.514889    -0.711879     109.55
 O       7.190131     0.818098    -0.858931     246.74
 H       7.273826     1.081941     0.082481      33.30
 H       6.825691    -0.900670    -1.673743      33.76
 H       7.202685    -1.108691    -0.015727      31.30
55
name= lig-ACN-Water-frame_179
 C      -3.986468     0.134725    -3.360134      51.39
 H      -4.263597    -0.718311    -3.925372      21.15
 C      -3.550256     1.515596    -1.287313      56.74
 H      -3.321393     1.565567    -0.240695      22.50
 C      -3.673027     2.713465    -2.015753       4.02
 O      -3.523638     3.960838    -1.404204     213.79
 C      -3.267018     4.039950    -0.010765     119.69
 H      -2.230217     3.504510     0.261529      24.59
 H      -4.022917     3.592365     0.485262      27.22
 H      -3.222950     5.109127     0.184364      25.53
 C      -3.706687     2.622066    -3.495834       9.17
 O      -3.589985     3.695899    -4.336330     131.60
 H      -3.435828     4.611408    -3.982995      19.24
 C      -3.866406     1.362830    -4.098313      58.17
 H      -3.864397     1.316925    -5.145759      24.79
 C      -3.768929     0.225797    -1.963849       1.00
 C      -3.667130    -1.150361    -1.155777      80.87
 H      -4.096154    -1.895165    -1.710386      29.61
 O      -4.462557    -1.004668     0.073084     176.69
 H      -4.077638    -0.559979     0.821522      28.30
 C      -2.202139    -1.808140    -0.867678      79.36
 H      -1.896746    -1.878492    -2.021705      27.29
 C      -2.204546    -3.206730    -0.156354     123.29
 O      -2.747539    -4.238248    -1.028036     201.41
 H      -2.452868    -4.099617    -2.018127      26.45
 H      -2.720472    -2.949598     0.720517      28.05
 H      -1.211342    -3.338446     0.121907      28.89
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 C       2.090401    -1.205428    -1.682581      65.95
 H       2.616228    -1.859175    -2.373989      17.26
 C       2.059947     0.555507    -0.016692      63.47
 H       2.496713     1.301506     0.499657      15.72
 C       0.737906     0.258297     0.297588      18.68
 O       0.017030     0.897541     1.310903     204.07
 C       0.649783     1.457193     2.536279     101.20
 H      -0.276060     1.713035     3.094825      23.70
 H       1.285322     0.854137     3.110229      26.71
 H       1.427727     2.357462     2.212522      22.31
 C       0.039504    -0.644083    -0.548235      15.90
 O      -1.319755    -0.987655    -0.047928     164.51
 C       0.668156    -1.384005    -1.521646     104.00
 H       0.353792    -2.293939    -2.071475      20.24
 C       2.721113    -0.160510    -1.065834      27.30
 C       4.139427     0.124335    -1.416789      89.12
 H       4.458615    -0.186185    -2.406340      22.56
 O       4.400238     1.581731    -1.387304     236.80
 H       4.883960     1.894317    -0.496784      20.54
 C       5.136553    -0.589647    -0.419531      87.59
 H       4.974157    -0.196773     0.600650      25.17
 O       4.874056    -2.007677    -0.367988     329.44
 H       4.826594    -2.346333    -1.256507      30.77
 C       6.595514    -0.536303    -0.780897     104.06
 O       7.147762     0.818125    -0.913229     247.19
 H       7.332826     1.335001    -0.036180      31.42
 H       6.636029    -1.013417    -1.747428      34.25
 H       7.101579    -1.123522    -0.064736      32.01
55
name= lig-ACN-Water-frame_180
 C      -3.981805     0.248015    -3.282446      59.41
 H      -4.144415    -0.740069    -3.708796      34.28
 C      -3.545704     1.462754    -1.330274      70.08
 H      -3.450759     1.536399    -0.307469      26.53
 C      -3.607031     2.686071    -2.058669       7.11
 O      -3.527264     3.997163    -1.422752     187.77
 C      -3.318818     4.030586     0.054469     118.04
 H      -2.286355     3.563182     0.406224      26.37
 H      -4.106240     3.650870     0.580826      28.21
 H      -3.304704     5.037224     0.299093      28.48
 C      -3.711889     2.635205    -3.488332       6.06
 O      -3.662928     3.697277    -4.393406     138.90
 H      -3.613693     4.544884    -3.804705      22.81
 C      -3.842477     1.341643    -4.103020      52.98
 H      -3.920679     1.257658    -5.204392      13.68
 C      -3.695111     0.197103    -1.890247      -1.86
 C      -3.599887    -1.108469    -1.091760      85.94
 H      -4.091261    -1.842568    -1.642939      27.46
 O      -4.461690    -1.111276     0.122093     159.28
 H      -3.800790    -0.669133     0.773975      27.22
 C      -2.194701    -1.750849    -0.887368      89.18
 H      -1.616441    -1.975873    -1.852157      25.74
 C      -2.277872    -3.154570    -0.161083     113.05
 O      -2.715421    -4.305704    -1.061615     166.77
 H      -2.275397    -4.185091    -1.969910      28.99
 H      -2.941582    -3.393027     0.600352      26.46
 H      -1.299526    -3.447775     0.141545      27.97
 C       2.052726    -1.180949    -1.696925      47.99
 H       2.603120    -1.711786    -2.476396      20.35
 C       2.094387     0.570812    -0.037365      69.65
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 H       2.673094     1.158328     0.634987      21.02
 C       0.754703     0.234519     0.255718      12.13
 O       0.035891     0.832486     1.312696     202.89
 C       0.699871     1.405030     2.492578     106.41
 H      -0.071231     1.803837     3.222848      25.09
 H       1.255048     0.619385     2.925985      27.08
 H       1.221140     2.464468     2.228249      24.03
 C      -0.047824    -0.731925    -0.485458      18.38
 O      -1.270038    -0.970259    -0.066507     189.55
 C       0.684843    -1.420772    -1.502424      66.62
 H       0.078398    -2.071557    -2.036500      23.08
 C       2.761261    -0.076830    -1.099246      35.11
 C       4.235559     0.133524    -1.384617      89.98
 H       4.354908    -0.286091    -2.430342      27.20
 O       4.341600     1.579941    -1.489864     202.59
 H       4.599319     1.895892    -0.505341      22.84
 C       5.156660    -0.604508    -0.451638      89.60
 H       5.035047    -0.245648     0.621783      26.28
 O       4.834850    -2.001084    -0.410426     305.65
 H       4.795701    -2.347561    -1.354134      30.16
 C       6.638038    -0.499695    -0.870315     109.78
 O       7.120763     0.823872    -0.962669     238.05
 H       7.333015     0.985266    -0.008249      31.22
 H       6.826659    -0.981904    -1.857353      33.22
 H       7.215446    -1.055420    -0.171179      32.21
55
name= lig-ACN-Water-frame_181
 C      -3.913103     0.160625    -3.232726      45.62
 H      -4.001355    -0.769026    -3.827313      31.63
 C      -3.530305     1.520911    -1.258644      57.72
 H      -3.437769     1.551548    -0.217008      26.30
 C      -3.524715     2.703108    -2.061451       9.79
 O      -3.530301     3.950047    -1.462620     169.20
 C      -3.408772     4.044681     0.062857     108.08
 H      -2.449282     3.460125     0.341912      27.66
 H      -4.205912     3.485306     0.492453      27.15
 H      -3.298842     5.023701     0.241469      28.59
 C      -3.685879     2.639627    -3.517822      21.29
 O      -3.743091     3.725156    -4.363340     136.88
 H      -3.515713     4.677811    -3.961061      22.04
 C      -3.866667     1.381520    -4.061612      38.05
 H      -4.098272     1.372779    -5.202112      12.94
 C      -3.638020     0.197249    -1.851167     -16.70
 C      -3.609616    -1.123042    -1.070749      72.37
 H      -4.072667    -1.787934    -1.784378      24.66
 O      -4.382793    -1.185784     0.187655     112.96
 H      -3.994477    -0.719866     1.019301      24.06
 C      -2.200062    -1.787601    -0.865011      85.78
 H      -1.910548    -1.804517    -1.940140      27.32
 C      -2.333794    -3.227985    -0.230655     129.23
 O      -2.673325    -4.295862    -1.089881     227.13
 H      -2.196527    -4.329826    -1.902513      28.88
 H      -3.049131    -2.985855     0.516217      26.29
 H      -1.437956    -3.299634     0.428802      26.33
 C       2.017546    -1.099352    -1.827866      67.05
 H       2.391753    -1.694454    -2.663780      23.04
 C       2.091089     0.551339    -0.019590      79.68
 H       2.590337     1.425805     0.530136      19.80
 C       0.739239     0.267317     0.307933      18.01
 O       0.005283     0.784941     1.329703     224.50
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 C       0.736080     1.339745     2.413444     107.48
 H      -0.095774     1.502267     3.148182      25.19
 H       1.485778     0.672238     2.867280      26.92
 H       1.455184     2.212805     2.114456      24.01
 C       0.089673    -0.766003    -0.418961       6.29
 O      -1.362708    -0.907564    -0.049567     118.48
 C       0.693497    -1.491345    -1.459692      66.76
 H       0.330080    -2.154110    -2.110584      22.46
 C       2.728698    -0.180758    -1.067624      45.21
 C       4.186624     0.191897    -1.444093      75.30
 H       4.512571    -0.186841    -2.500285      24.15
 O       4.379400     1.607239    -1.571267     232.00
 H       4.466365     2.017066    -0.683397      27.38
 C       5.217322    -0.639367    -0.476838      92.92
 H       5.114707    -0.252981     0.615413      25.18
 O       4.769026    -2.047609    -0.452883     295.41
 H       4.856331    -2.428630    -1.417104      27.62
 C       6.725931    -0.547904    -0.948903      96.61
 O       7.126877     0.891124    -0.966348     246.82
 H       7.459552     1.240001    -0.158795      32.66
 H       6.735429    -0.889946    -2.047176      32.43
 H       7.346726    -1.156390    -0.294475      30.17
55
name= lig-ACN-Water-frame_182
 C      -3.782114     0.168263    -3.266900      49.72
 H      -3.936016    -0.840550    -3.729709      17.51
 C      -3.483042     1.532043    -1.215128      65.65
 H      -3.370738     1.733340    -0.132848      20.89
 C      -3.496433     2.690796    -2.015416       9.48
 O      -3.513683     3.946577    -1.453981     222.75
 C      -3.487090     3.999725    -0.070346     134.23
 H      -2.598635     3.527505     0.424076      26.81
 H      -4.450661     3.728903     0.448429      26.89
 H      -3.516840     4.996942     0.142740      27.74
 C      -3.650941     2.641965    -3.443683      -1.93
 O      -3.810637     3.771273    -4.307601     165.33
 H      -3.581856     4.628561    -3.757413      17.79
 C      -3.913323     1.327401    -3.977913      48.70
 H      -4.122246     1.181352    -5.138220      28.82
 C      -3.634743     0.255186    -1.833790      17.09
 C      -3.632286    -1.167959    -1.034004      86.07
 H      -4.254434    -1.942377    -1.521831      25.75
 O      -4.335881    -1.221846     0.248830     153.82
 H      -3.815439    -0.581189     0.763695      27.54
 C      -2.214965    -1.801664    -0.932937      86.10
 H      -1.687570    -1.895213    -1.844631      25.88
 C      -2.324244    -3.166456    -0.199776     109.76
 O      -2.653507    -4.309535    -1.127598     168.03
 H      -2.243354    -4.086307    -2.007467      29.61
 H      -3.222479    -3.307593     0.403624      25.19
 H      -1.417879    -3.608411     0.298883      25.00
 C       1.992502    -1.093599    -1.919781      41.44
 H       2.557288    -1.414082    -2.801113      21.66
 C       2.073395     0.500396    -0.010996      61.32
 H       2.619493     1.498606     0.374200      17.40
 C       0.748037     0.188285     0.328083      12.99
 O      -0.040541     0.766286     1.337130     209.23
 C       0.803080     1.288046     2.419789     103.96
 H       0.181427     1.666726     3.264316      25.46
 H       1.495856     0.450623     2.740240      25.43
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 H       1.205504     2.246859     2.070548      24.22
 C       0.023090    -0.836500    -0.369108       6.00
 O      -1.362826    -0.863840    -0.070746     132.23
 C       0.704514    -1.520404    -1.436786      62.50
 H       0.117322    -2.265286    -1.815261      21.76
 C       2.732910    -0.198421    -1.064745      34.61
 C       4.157721     0.151832    -1.484253      55.74
 H       4.199030    -0.229455    -2.632653      19.67
 O       4.456824     1.668529    -1.605965     226.35
 H       4.710239     1.943711    -0.736491      26.77
 C       5.257673    -0.678039    -0.570770      85.40
 H       5.181046    -0.328706     0.554920      23.17
 O       4.737151    -2.060176    -0.507147     298.19
 H       4.887468    -2.488590    -1.386678      29.68
 C       6.720961    -0.507072    -1.000191     102.17
 O       7.158845     0.931787    -0.993004     249.22
 H       7.312621     1.031961     0.010099      30.65
 H       6.861959    -0.792567    -2.128856      30.68
 H       7.497246    -1.131996    -0.454293      29.15
55
name= lig-ACN-Water-frame_183
 C      -3.710824     0.175138    -3.152390      26.18
 H      -3.799244    -0.789754    -3.685951      18.79
 C      -3.442253     1.469276    -1.216970      52.28
 H      -3.384786     1.394818    -0.062717      20.93
 C      -3.511182     2.660418    -2.015752      14.28
 O      -3.469419     3.971698    -1.517418     215.66
 C      -3.600405     4.078816    -0.045446     106.04
 H      -2.810544     3.542974     0.427368      26.84
 H      -4.541911     3.443861     0.217770      24.78
 H      -3.434551     5.118766     0.154525      25.65
 C      -3.704481     2.609622    -3.413246       9.85
 O      -3.847032     3.734899    -4.174418     164.23
 H      -3.823362     4.598329    -3.690705      19.69
 C      -3.857922     1.360412    -4.000047      46.75
 H      -4.043869     1.372273    -5.162225      24.37
 C      -3.631871     0.166720    -1.775664      33.49
 C      -3.656075    -1.158823    -1.052468      88.96
 H      -4.205693    -1.793227    -1.836309      25.23
 O      -4.265389    -1.147949     0.299176     175.85
 H      -3.744578    -0.701492     0.975103      24.85
 C      -2.196702    -1.800535    -0.895199      88.89
 H      -1.889359    -1.942857    -1.866842      27.14
 C      -2.302858    -3.224572    -0.200989     103.55
 O      -2.636815    -4.291919    -1.204667     183.76
 H      -2.415229    -4.065481    -2.203523      25.20
 H      -2.958315    -3.150042     0.730419      24.81
 H      -1.272803    -3.182285     0.319778      24.90
 C       1.969507    -1.121295    -1.827093      65.16
 H       2.244579    -1.658903    -2.738729      16.77
 C       2.047352     0.434540    -0.020435      65.81
 H       2.649914     1.198262     0.706281      18.00
 C       0.707721     0.077678     0.364449      11.91
 O      -0.027939     0.773640     1.366473     221.48
 C       0.824591     1.301282     2.440932     111.70
 H       0.144512     1.401601     3.285242      24.60
 H       1.634643     0.505640     2.728659      25.83
 H       1.453927     2.084815     2.164996      26.00
 C      -0.009596    -0.876847    -0.401517      16.61
 O      -1.346298    -0.916916    -0.159969     163.45
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 C       0.667250    -1.530466    -1.434402      61.17
 H       0.298252    -2.292591    -2.127157      18.93
 C       2.706666    -0.121433    -1.149131      54.70
 C       4.205922     0.164286    -1.515574      74.88
 H       4.391807    -0.234060    -2.673468      22.07
 O       4.505290     1.600673    -1.592353     229.05
 H       4.969495     1.891705    -0.722962      21.55
 C       5.173956    -0.669701    -0.691056      79.05
 H       5.096612    -0.235610     0.409709      20.79
 O       4.782134    -2.056132    -0.581957     318.08
 H       4.788062    -2.448616    -1.460109      29.02
 C       6.731803    -0.420212    -1.142753      81.28
 O       7.181606     0.904724    -0.964897     278.47
 H       7.249746     1.211988     0.032067      29.13
 H       6.860646    -0.795396    -2.259704      29.60
 H       7.225946    -1.110141    -0.353654      28.39
55
name= lig-ACN-Water-frame_184
 C      -3.749564     0.161080    -3.223079      70.91
 H      -3.716280    -0.787452    -3.728345      28.85
 C      -3.449700     1.439800    -1.162210      59.18
 H      -3.279214     1.709468    -0.044276      18.67
 C      -3.525192     2.608091    -1.938749       5.86
 O      -3.413067     3.966013    -1.526770     221.74
 C      -3.665983     4.116290    -0.054903     106.16
 H      -2.925536     3.686753     0.499031      28.83
 H      -4.756253     3.788984     0.307680      26.04
 H      -3.839383     5.246699     0.135179      25.34
 C      -3.775575     2.566061    -3.354707      17.61
 O      -3.884887     3.711496    -4.089653     180.61
 H      -3.663899     4.487848    -3.574859      23.89
 C      -3.731758     1.309855    -3.983170      54.63
 H      -3.847498     1.157759    -5.088097      14.04
 C      -3.586234     0.191141    -1.784266      20.73
 C      -3.589339    -1.149508    -0.980327      80.96
 H      -4.303383    -1.982856    -1.387870      22.33
 O      -4.249798    -1.068148     0.295475     201.34
 H      -3.539372    -0.602051     0.804460      25.44
 C      -2.275849    -1.873849    -0.934097     100.57
 H      -1.918568    -1.950919    -1.894601      27.55
 C      -2.189076    -3.236791    -0.284347     119.73
 O      -2.641988    -4.238120    -1.200578     197.89
 H      -2.235491    -3.957600    -2.060964      29.00
 H      -2.971724    -3.388521     0.532241      24.76
 H      -1.196290    -3.701769     0.000125      24.88
 C       1.993680    -1.185165    -1.759773      86.81
 H       2.597796    -1.702563    -2.511437      16.38
 C       2.032557     0.366045     0.009577      55.54
 H       2.620903     1.070863     0.747147      16.64
 C       0.716594     0.058551     0.374502      12.60
 O       0.053496     0.752687     1.387540     236.59
 C       0.846165     1.266014     2.478283     119.14
 H       0.155317     1.538186     3.257011      25.67
 H       1.596290     0.463670     2.903237      23.91
 H       1.196621     2.172659     2.253370      26.52
 C      -0.013897    -0.879317    -0.454841       6.60
 O      -1.388076    -0.983313    -0.212304     163.82
 C       0.649438    -1.554480    -1.488191      64.63
 H      -0.017064    -2.226483    -2.178021      19.24
 C       2.667215    -0.099158    -1.196795      30.60
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 C       4.137865     0.175658    -1.625544      71.29
 H       4.282265    -0.169858    -2.816613      20.90
 O       4.547714     1.522633    -1.563111     231.24
 H       4.942137     1.748331    -0.623248      19.31
 C       5.175722    -0.601636    -0.761657      64.01
 H       5.104627    -0.268303     0.365929      21.51
 O       4.860230    -2.040161    -0.685889     349.94
 H       4.764959    -2.362823    -1.652621      26.12
 C       6.630936    -0.445513    -1.158461      94.84
 O       7.221210     0.928316    -0.959576     276.67
 H       7.412744     0.962904     0.021781      30.40
 H       6.844575    -0.568736    -2.312207      29.09
 H       7.351102    -1.234818    -0.677589      28.54
55
name= lig-ACN-Water-frame_185
 C      -3.743584     0.057820    -3.200492      64.10
 H      -3.813495    -0.897281    -3.661263      32.00
 C      -3.466405     1.464245    -1.115995      45.84
 H      -3.234886     1.354070    -0.024688      23.33
 C      -3.563921     2.630683    -1.904458      21.60
 O      -3.383559     3.893441    -1.410600     229.48
 C      -3.758073     4.218918    -0.104409      98.37
 H      -3.089224     3.941752     0.608527      29.07
 H      -4.763251     3.594488     0.106575      24.35
 H      -3.665684     5.418220    -0.126564      24.18
 C      -3.746025     2.515034    -3.303162       6.48
 O      -3.906664     3.692348    -4.059276     187.29
 H      -3.686436     4.539195    -3.576616      24.46
 C      -3.673609     1.271313    -4.005971      48.14
 H      -3.610410     1.348426    -5.062100      14.39
 C      -3.567948     0.181729    -1.815990     -29.43
 C      -3.653909    -1.201953    -0.966077      64.55
 H      -4.357590    -1.796060    -1.716808      22.87
 O      -4.239447    -0.971925     0.327718     182.33
 H      -3.735268    -0.453884     1.009009      23.21
 C      -2.197124    -1.905495    -1.008153      86.42
 H      -1.977183    -1.984237    -2.019831      28.77
 C      -2.137304    -3.308946    -0.320091     117.25
 O      -2.705504    -4.238530    -1.281756     206.68
 H      -2.234755    -4.387688    -2.089634      28.60
 H      -2.706061    -3.302285     0.663191      25.13
 H      -1.079124    -3.216173     0.135294      24.78
 C       2.033839    -1.275318    -1.844292      69.54
 H       2.529353    -1.841031    -2.639539      15.92
 C       2.082929     0.377880     0.023358      60.48
 H       2.588359     1.250737     0.477035      20.22
 C       0.741520     0.047721     0.325863      -0.73
 O       0.097167     0.667038     1.414251     207.07
 C       0.822822     1.284632     2.546413     115.27
 H       0.067205     1.430390     3.286668      25.51
 H       1.650894     0.556819     2.940939      25.22
 H       1.346894     2.052189     2.251565      27.51
 C      -0.054459    -0.864103    -0.475655       4.04
 O      -1.378072    -0.988935    -0.201484     149.88
 C       0.661947    -1.546790    -1.512258      59.50
 H       0.134074    -2.442363    -2.152614      21.91
 C       2.651935    -0.193613    -1.126874      24.65
 C       4.058838     0.143872    -1.646481      58.95
 H       4.015478    -0.148486    -2.858986      21.34
 O       4.554421     1.563413    -1.558763     232.41
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 H       4.794276     1.691580    -0.647136      27.72
 C       5.157156    -0.646032    -0.788248      61.96
 H       4.931343    -0.228247     0.275607      25.37
 O       4.924644    -2.018304    -0.808767     327.69
 H       5.125630    -2.421993    -1.764601      28.43
 C       6.645855    -0.369088    -1.240605      79.92
 O       7.246899     0.903792    -0.951712     307.78
 H       7.529157     1.011556    -0.052390      30.75
 H       6.525178    -0.565432    -2.385898      29.20
 H       7.225009    -1.213091    -0.694289      28.94
55
name= lig-ACN-Water-frame_186
 C      -3.682519     0.069383    -3.186214      54.00
 H      -3.794554    -0.888002    -3.656520      23.92
 C      -3.478094     1.350359    -1.158357      60.03
 H      -3.390843     1.535438    -0.115115      23.51
 C      -3.577757     2.564190    -1.852759     -42.17
 O      -3.327366     3.853728    -1.379705     201.45
 C      -3.844181     4.311872    -0.065914     106.25
 H      -3.202286     4.015734     0.673325      27.33
 H      -4.965576     3.993810     0.206917      23.84
 H      -4.093061     5.524287    -0.152800      23.03
 C      -3.662135     2.529562    -3.314162      -7.52
 O      -3.904272     3.638492    -4.064729     165.00
 H      -3.666051     4.512571    -3.535482      16.48
 C      -3.680115     1.266995    -3.955357      77.66
 H      -3.712305     1.222707    -4.976344      28.59
 C      -3.617335     0.112542    -1.764749      40.71
 C      -3.645617    -1.130120    -1.034229      77.87
 H      -4.423021    -1.984642    -1.372758      23.66
 O      -4.290346    -0.957004     0.333750     146.76
 H      -3.484077    -0.641459     0.857470      27.65
 C      -2.229927    -1.860960    -0.989992      96.08
 H      -1.764566    -1.855293    -1.949532      28.14
 C      -2.120866    -3.258032    -0.389782     117.10
 O      -2.770556    -4.316472    -1.303599     163.02
 H      -2.192844    -4.208429    -2.137546      28.79
 H      -2.751188    -3.352543     0.494283      27.41
 H      -1.206909    -3.795661    -0.267354      25.93
 C       1.995753    -1.278179    -1.860200      38.44
 H       2.383534    -1.782505    -2.736004      23.49
 C       2.084760     0.395946    -0.061003      69.23
 H       2.504745     1.205895     0.418268      22.12
 C       0.759587     0.075675     0.350953      13.27
 O       0.076931     0.561031     1.451636     206.55
 C       0.828286     1.257447     2.542040     117.98
 H       0.051279     1.530851     3.238206      26.65
 H       1.500121     0.517737     3.052969      27.03
 H       1.202193     2.137195     2.297078      28.98
 C       0.060152    -0.855105    -0.506174       4.37
 O      -1.361160    -0.982595    -0.191885     151.60
 C       0.678700    -1.570661    -1.506553      66.07
 H       0.116793    -2.447119    -2.138075      21.17
 C       2.724541    -0.339633    -1.139501      39.37
 C       4.090613     0.164371    -1.571102      78.91
 H       4.313488    -0.079244    -2.763499      20.77
 O       4.467269     1.579796    -1.579670     231.88
 H       4.646216     1.952043    -0.700671      26.57
 C       5.131095    -0.615539    -0.864561     101.25
 H       5.079357    -0.465473     0.270741      23.89
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 O       4.970521    -2.084297    -0.912749     275.59
 H       5.188115    -2.381619    -1.869640      28.42
 C       6.625949    -0.318335    -1.304227      97.04
 O       7.279756     0.918567    -0.985570     296.16
 H       7.409777     0.933922    -0.002824      30.75
 H       6.885208    -0.372794    -2.416136      29.22
 H       7.249308    -1.143867    -0.868244      29.06
55
name= lig-ACN-Water-frame_187
 C      -3.652959     0.095070    -3.184240      57.29
 H      -3.652347    -0.848973    -3.753209      24.74
 C      -3.521290     1.348176    -1.107354      53.45
 H      -3.523378     1.281896    -0.074801      21.94
 C      -3.514221     2.523993    -1.899556     -20.46
 O      -3.316051     3.847399    -1.322484     179.55
 C      -3.968786     4.368005    -0.060450      91.15
 H      -3.326284     4.191054     0.814655      25.30
 H      -4.981982     3.834621     0.103143      23.67
 H      -3.806926     5.572552    -0.245722      22.87
 C      -3.633231     2.507434    -3.290318       7.95
 O      -3.861034     3.628347    -4.092257     152.12
 H      -3.522864     4.498135    -3.651638      19.36
 C      -3.702216     1.267081    -3.917414      78.76
 H      -3.906526     1.219642    -4.931107      26.51
 C      -3.677364     0.088822    -1.800431     -30.17
 C      -3.655067    -1.231742    -0.929460      87.35
 H      -4.239444    -2.006252    -1.674170      24.49
 O      -4.270092    -0.993124     0.303226     207.32
 H      -3.737336    -0.542753     1.071655      22.20
 C      -2.199498    -1.775890    -0.968958      80.83
 H      -2.064988    -1.780504    -2.062055      27.87
 C      -2.237411    -3.338458    -0.487163     124.44
 O      -2.804318    -4.323737    -1.311784     215.46
 H      -2.692514    -4.215891    -2.328308      27.38
 H      -2.664231    -3.385958     0.479233      26.91
 H      -1.174860    -3.324051    -0.281204      26.80
 C       2.021463    -1.289367    -1.889290      22.63
 H       2.569491    -1.736011    -2.711064      19.57
 C       2.074637     0.390823    -0.115283      85.30
 H       2.689887     0.981323     0.392892      21.49
 C       0.788023     0.049418     0.326797      19.80
 O       0.072604     0.487044     1.489630     216.31
 C       0.764916     1.223646     2.515923     123.30
 H       0.001831     1.487685     3.245583      25.67
 H       1.551759     0.666663     2.992994      27.19
 H       1.245067     1.994542     2.046088      27.53
 C       0.016961    -0.886470    -0.436187      15.42
 O      -1.287299    -0.960804    -0.159053     176.19
 C       0.662114    -1.608896    -1.503907      69.42
 H      -0.076732    -2.237532    -2.165636      20.00
 C       2.730370    -0.269072    -1.157001      44.91
 C       4.167163     0.144851    -1.600725      61.46
 H       4.142284    -0.184340    -2.772743      20.81
 O       4.336127     1.591008    -1.576952     221.92
 H       4.405116     1.800656    -0.550378      22.87
 C       5.308411    -0.673641    -0.849790      91.25
 H       5.244486    -0.392091     0.232974      23.75
 O       4.992616    -2.100274    -1.002582     340.43
 H       4.930126    -2.447030    -1.943380      28.69
 C       6.677934    -0.337687    -1.380311     100.10
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 O       7.288680     1.001835    -0.994177     278.16
 H       7.682044     0.955361    -0.017817      28.28
 H       6.521400    -0.410665    -2.476636      33.29
 H       7.282885    -1.111747    -0.972661      31.13
55
name= lig-ACN-Water-frame_188
 C      -3.691408     0.027762    -3.186342      67.28
 H      -3.692524    -0.987252    -3.683237      25.37
 C      -3.614884     1.347267    -1.099807      52.70
 H      -3.503546     1.492086    -0.051360      23.01
 C      -3.441870     2.598480    -1.782636       9.02
 O      -3.326228     3.832672    -1.275855     226.24
 C      -3.992700     4.323268    -0.140785     107.61
 H      -3.495288     3.989494     0.842426      25.02
 H      -5.085506     4.019034    -0.080590      25.53
 H      -4.175474     5.508448    -0.284969      23.81
 C      -3.649666     2.539172    -3.286366     -14.26
 O      -3.774905     3.648367    -4.110304     141.38
 H      -3.520046     4.479125    -3.677889      22.86
 C      -3.740193     1.271665    -3.981186      59.19
 H      -3.769571     1.350906    -5.073967      20.96
 C      -3.680724     0.094685    -1.743745      26.71
 C      -3.619846    -1.183126    -0.953106      79.02
 H      -4.332742    -2.089273    -1.332140      22.66
 O      -4.285922    -1.077875     0.363917     162.83
 H      -3.581704    -0.547794     0.853275      28.27
 C      -2.251633    -1.828708    -0.956242      95.97
 H      -1.725864    -1.706926    -1.944920      26.17
 C      -2.186579    -3.274669    -0.482396     122.31
 O      -2.860119    -4.312852    -1.371459     191.87
 H      -2.452731    -4.146075    -2.239461      30.18
 H      -2.721776    -3.391190     0.401671      27.88
 H      -1.245217    -3.780026    -0.378446      26.80
 C       2.014269    -1.269349    -1.859470     -13.04
 H       2.344352    -1.899469    -2.673453      14.17
 C       2.107595     0.397224    -0.032919      75.14
 H       2.513751     1.118234     0.583603      17.81
 C       0.776689    -0.013409     0.348497      10.26
 O       0.089752     0.397287     1.473303     224.95
 C       0.753402     1.233611     2.459676     123.18
 H      -0.019238     1.583552     3.164442      25.69
 H       1.426924     0.700143     3.010029      28.16
 H       1.162542     2.168440     2.121222      26.47
 C       0.074327    -0.952921    -0.469564      10.47
 O      -1.354328    -0.997774    -0.119316     150.05
 C       0.690140    -1.556399    -1.523759      76.50
 H       0.233223    -2.273685    -2.215544      21.41
 C       2.703512    -0.243007    -1.259372      55.81
 C       4.157783     0.084327    -1.632625      76.71
 H       4.433551    -0.100833    -2.773217      21.95
 O       4.240746     1.539407    -1.538672     227.05
 H       4.581989     1.896108    -0.596514      20.98
 C       5.348879    -0.709856    -0.852489      73.03
 H       5.320331    -0.578643     0.233424      26.99
 O       5.009303    -2.068241    -1.005625     396.34
 H       5.303962    -2.269711    -1.921264      31.91
 C       6.837139    -0.309592    -1.435444     119.05
 O       7.255031     1.019551    -1.042878     315.38
 H       7.733213     0.903648    -0.129228      29.21
 H       6.809890    -0.183701    -2.493783      34.28
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 H       7.588426    -1.011921    -1.286407      31.91
55
name= lig-ACN-Water-frame_189
 C      -3.781817     0.098692    -3.173939     108.35
 H      -3.828612    -0.927551    -3.641704      35.10
 C      -3.633606     1.417006    -1.079687      33.55
 H      -3.651540     1.379017     0.031332      27.61
 C      -3.531525     2.552075    -1.879739      20.80
 O      -3.267913     3.874518    -1.293224     216.26
 C      -4.124977     4.263501    -0.157592      94.87
 H      -3.623513     3.920351     0.896684      25.05
 H      -5.108256     3.799287    -0.243763      25.86
 H      -3.951403     5.414104    -0.133354      24.65
 C      -3.645209     2.520526    -3.256755      16.01
 O      -3.664126     3.673745    -4.091450     102.36
 H      -3.597709     4.524073    -3.635360      24.75
 C      -3.736735     1.248761    -3.891822      52.19
 H      -3.675871     1.136734    -5.027484      18.56
 C      -3.686510     0.154306    -1.767821     -67.58
 C      -3.695658    -1.195363    -0.971629      35.64
 H      -4.396850    -1.871726    -1.668119      19.37
 O      -4.217726    -1.126129     0.440468     132.12
 H      -3.703654    -0.685152     1.117823      27.14
 C      -2.163955    -1.876528    -0.971818      70.93
 H      -1.954963    -1.925230    -2.106334      27.38
 C      -2.160335    -3.362472    -0.436706     118.10
 O      -2.869834    -4.200901    -1.442854     197.03
 H      -2.297509    -4.429649    -2.172986      28.82
 H      -2.633118    -3.355915     0.502825      26.04
 H      -1.106541    -3.512265    -0.269683      26.19
 C       2.022299    -1.247885    -1.888154      15.14
 H       2.624134    -1.696047    -2.685422      17.31
 C       2.102595     0.307681    -0.039707      75.50
 H       2.668343     1.164231     0.375971      20.75
 C       0.831870    -0.091320     0.349200      14.95
 O       0.120602     0.350515     1.470034     202.79
 C       0.724919     1.269984     2.441553     114.83
 H      -0.158400     1.506452     3.044604      25.89
 H       1.460260     0.821720     2.969826      28.54
 H       1.150838     2.132971     1.859382      26.50
 C      -0.017409    -0.951956    -0.441405      -7.35
 O      -1.362420    -1.076805    -0.083016     155.92
 C       0.656841    -1.582607    -1.582779      66.24
 H       0.125206    -2.299121    -2.065259      24.12
 C       2.733395    -0.230352    -1.160832      35.99
 C       4.181076     0.110402    -1.602976      84.49
 H       4.222328    -0.257891    -2.716182      22.51
 O       4.219499     1.525231    -1.508880     246.06
 H       4.810696     1.689495    -0.739343      22.74
 C       5.368472    -0.659079    -0.904422      82.69
 H       5.396779    -0.358371     0.130734      26.22
 O       5.071320    -2.092979    -0.994690     357.55
 H       5.186508    -2.508853    -1.860706      31.81
 C       6.886651    -0.266986    -1.507945     103.46
 O       7.259069     1.041806    -1.063546     374.55
 H       7.521690     1.095070    -0.137084      32.27
 H       6.769844    -0.275583    -2.530337      33.77
 H       7.502337    -0.991244    -1.119311      31.47
55
name= lig-ACN-Water-frame_190
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 C      -3.855088     0.118457    -3.065620      43.07
 H      -3.989025    -0.825783    -3.618371      29.17
 C      -3.621804     1.419771    -1.095746      53.64
 H      -3.588226     1.544514     0.051554      23.71
 C      -3.618042     2.647896    -1.863456      -6.53
 O      -3.263966     3.847088    -1.350464     196.69
 C      -4.170356     4.195105    -0.148274      99.95
 H      -3.777834     3.582173     0.860615      22.77
 H      -5.179006     3.902894    -0.343533      25.48
 H      -4.264124     5.280238    -0.074139      25.20
 C      -3.642725     2.567479    -3.315982       8.95
 O      -3.550943     3.650628    -4.063737      48.02
 H      -3.534829     4.486444    -3.482577      21.55
 C      -3.725549     1.291331    -3.901696       1.97
 H      -3.837048     1.306841    -5.077715      13.03
 C      -3.743857     0.148981    -1.667624      26.59
 C      -3.643569    -1.194659    -0.915695      67.42
 H      -4.382181    -1.977099    -1.343340      22.45
 O      -4.155774    -1.165098     0.424751     155.55
 H      -3.397014    -0.707029     0.891115      28.19
 C      -2.271293    -1.914212    -0.968995      86.40
 H      -1.733562    -1.816398    -1.986019      26.81
 C      -2.161108    -3.376489    -0.460181     126.17
 O      -2.841219    -4.105685    -1.443639     222.27
 H      -2.222500    -4.260800    -2.257905      26.85
 H      -2.672212    -3.660549     0.452239      26.39
 H      -1.178384    -3.797685    -0.349739      26.94
 C       1.990327    -1.222991    -1.902783      63.05
 H       2.367924    -1.721995    -2.808606      26.38
 C       2.107939     0.268478    -0.023864      53.47
 H       2.617340     1.049750     0.697490      19.26
 C       0.785725    -0.135706     0.371561      19.48
 O       0.148551     0.322290     1.499769     211.93
 C       0.692052     1.292962     2.383413     122.73
 H      -0.048341     1.669544     3.093641      26.38
 H       1.471810     0.939627     2.947934      28.07
 H       1.044341     2.276198     1.848486      25.91
 C       0.028447    -0.971188    -0.499654      20.12
 O      -1.313769    -1.154026    -0.092540     155.02
 C       0.634134    -1.581280    -1.571229      77.60
 H       0.177252    -2.100332    -2.296266      24.66
 C       2.771983    -0.407165    -1.104766      34.63
 C       4.127619     0.094223    -1.596701      85.27
 H       4.129153    -0.018472    -2.721201      22.64
 O       4.293896     1.581701    -1.516605     271.69
 H       4.706944     1.892580    -0.730258      24.15
 C       5.397234    -0.625524    -0.994017     106.89
 H       5.393685    -0.445220     0.044687      24.51
 O       5.153543    -2.090498    -0.949415     320.90
 H       5.063295    -2.209305    -1.932269      28.51
 C       6.756395    -0.280903    -1.474702     117.66
 O       7.283293     1.112203    -1.098276     284.67
 H       7.564191     1.042112    -0.176130      30.20
 H       6.931769    -0.311415    -2.506829      33.19
 H       7.426987    -0.984885    -1.091110      31.82
55
name= lig-ACN-Water-frame_191
 C      -3.905758     0.138646    -3.068911      84.77
 H      -4.060265    -0.841145    -3.479998      33.49
 C      -3.628227     1.464885    -1.060506      27.00
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 H      -3.298420     1.663313     0.028408      17.67
 C      -3.609365     2.585362    -1.865816       4.02
 O      -3.378478     3.891372    -1.296556     246.07
 C      -4.186743     4.128008    -0.199733     114.53
 H      -3.719449     3.569146     0.840591      23.41
 H      -5.147733     3.723731    -0.369603      27.07
 H      -4.051634     5.122378     0.036920      25.80
 C      -3.640859     2.546737    -3.262805      -6.04
 O      -3.443195     3.685764    -4.102507     -22.08
 H      -3.447801     4.667407    -3.666066      19.24
 C      -3.788037     1.280748    -3.876604      45.49
 H      -3.789064     1.134974    -5.040673      19.76
 C      -3.785362     0.143044    -1.622221     -76.65
 C      -3.618059    -1.243500    -0.881390      75.69
 H      -4.244367    -1.956392    -1.506971      23.89
 O      -4.063839    -1.134029     0.456811     210.40
 H      -3.482150    -0.818253     1.244742      20.98
 C      -2.196092    -1.884734    -0.899217      87.02
 H      -2.060063    -1.915323    -2.053838      27.53
 C      -2.191243    -3.358268    -0.489238     116.10
 O      -2.884424    -4.148450    -1.526123     196.49
 H      -2.402290    -3.952482    -2.422559      27.24
 H      -2.698716    -3.353681     0.503212      25.06
 H      -1.125256    -3.539358    -0.411990      26.95
 C       1.976422    -1.284110    -1.927314      43.72
 H       2.376902    -1.621236    -2.900224      20.59
 C       2.107766     0.152517     0.067160      81.53
 H       2.780030     0.855629     0.788718      19.53
 C       0.783983    -0.119636     0.367680      28.74
 O       0.097033     0.288444     1.538659     205.34
 C       0.717962     1.378028     2.363239     106.38
 H      -0.125240     1.538277     3.012410      24.48
 H       1.568940     1.029164     2.884569      25.46
 H       0.962240     2.327519     1.654565      23.64
 C       0.014078    -1.002603    -0.468510      19.24
 O      -1.276802    -1.182781    -0.095396     180.21
 C       0.644533    -1.551249    -1.648528      36.01
 H       0.020719    -2.141130    -2.275732      19.96
 C       2.762137    -0.439630    -1.069752     101.58
 C       4.146055     0.144782    -1.645028      62.21
 H       4.201775    -0.136199    -2.689677      24.38
 O       4.345132     1.615439    -1.551109     255.40
 H       4.553145     1.673899    -0.588557      25.66
 C       5.286452    -0.607624    -0.910020     116.77
 H       5.262248    -0.319395     0.089853      26.32
 O       5.218751    -2.025801    -0.994563     269.02
 H       5.278498    -2.500075    -1.878149      31.88
 C       6.790835    -0.208118    -1.449421      99.89
 O       7.279929     1.100084    -1.156802     288.54
 H       7.649521     1.188597    -0.186522      28.85
 H       6.685833    -0.311505    -2.541854      34.45
 H       7.380639    -0.990542    -1.002681      32.95
55
name= lig-ACN-Water-frame_192
 C      -3.959883     0.096784    -3.025981      95.19
 H      -4.020753    -0.787428    -3.579098      25.46
 C      -3.594309     1.410863    -0.998055      44.45
 H      -3.440304     1.345494     0.117163      18.24
 C      -3.540389     2.619608    -1.846205       0.42
 O      -3.472727     3.875059    -1.350193     212.44
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 C      -4.231616     4.113528    -0.085093     108.82
 H      -3.740353     3.481076     0.837212      24.31
 H      -5.271343     3.926088    -0.189145      27.26
 H      -4.228886     5.093980     0.047329      27.24
 C      -3.622040     2.579955    -3.316070      -4.87
 O      -3.358712     3.637217    -4.131973      28.57
 H      -3.506645     4.536116    -3.600530      18.79
 C      -3.869335     1.267842    -3.829695      14.59
 H      -3.793964     1.173667    -4.957892      21.51
 C      -3.758644     0.171299    -1.652260      14.98
 C      -3.575319    -1.161849    -0.839457      71.14
 H      -4.255234    -1.912508    -1.204618      23.43
 O      -4.059028    -1.116129     0.582944     195.84
 H      -3.278117    -0.690928     0.993828      25.89
 C      -2.165777    -1.842983    -0.995032      83.23
 H      -1.647475    -1.692663    -1.996996      23.15
 C      -2.223435    -3.338994    -0.564426     108.87
 O      -2.950502    -4.192863    -1.547044     216.95
 H      -2.456857    -4.219810    -2.387415      29.79
 H      -2.795076    -3.662622     0.377709      23.70
 H      -1.244531    -3.826540    -0.361670      25.56
 C       2.034793    -1.271986    -1.941578      34.66
 H       2.587932    -1.634517    -2.826152      15.82
 C       2.182756     0.011694     0.131501      67.02
 H       2.819541     0.791439     0.783904      16.37
 C       0.771690    -0.154129     0.421343      13.25
 O       0.083094     0.296622     1.565530     216.77
 C       0.681963     1.406903     2.318450     104.38
 H       0.094600     1.797786     3.136893      24.57
 H       1.689168     1.145914     2.728453      24.25
 H       0.855672     2.344274     1.555986      22.64
 C       0.062607    -1.003448    -0.480086      11.70
 O      -1.281330    -1.160752    -0.060619     206.90
 C       0.592079    -1.534726    -1.655850      91.34
 H       0.043562    -2.306161    -2.286191      21.11
 C       2.717396    -0.327920    -1.158080      27.70
 C       4.132433     0.129228    -1.640298      90.78
 H       4.172838    -0.057383    -2.660639      24.71
 O       4.337664     1.570468    -1.575341     206.69
 H       4.754623     1.935630    -0.702728      25.64
 C       5.324212    -0.531913    -0.841669     101.38
 H       5.117247    -0.441872     0.164678      31.53
 O       5.234930    -1.999261    -1.029272     326.59
 H       5.449386    -1.974543    -1.993798      30.11
 C       6.729156    -0.194994    -1.390317     111.02
 O       7.316317     1.124225    -1.219867     215.04
 H       7.548206     1.145611    -0.204494      28.49
 H       6.709490    -0.314254    -2.527619      33.50
 H       7.502414    -0.918038    -1.071735      32.72
55
name= lig-ACN-Water-frame_193
 C      -3.981067     0.087326    -3.036630      53.61
 H      -4.132857    -0.889642    -3.411232      32.82
 C      -3.549711     1.428389    -1.067902      55.84
 H      -3.660488     1.647022    -0.024430      20.26
 C      -3.525684     2.572162    -1.821002       1.73
 O      -3.581845     3.917684    -1.342949     188.25
 C      -4.274033     4.152080     0.000084     120.42
 H      -3.746546     3.594371     0.824563      24.51
 H      -5.253510     3.713280    -0.115200      26.53
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 H      -4.107344     5.108910     0.218099      26.45
 C      -3.587765     2.485853    -3.237933       9.72
 O      -3.322449     3.563450    -4.137916     100.87
 H      -3.279275     4.490277    -3.746801      17.84
 C      -3.901968     1.276639    -3.837821      69.66
 H      -3.996269     1.209655    -4.894723      27.27
 C      -3.704888     0.134982    -1.610704     -23.41
 C      -3.622768    -1.129253    -0.801320      73.51
 H      -4.307478    -1.779659    -1.262082      22.80
 O      -3.980043    -1.066886     0.626090     188.13
 H      -3.513035    -0.553580     1.279425      23.17
 C      -2.193924    -1.819528    -1.009412      78.96
 H      -1.981001    -1.673074    -2.084367      26.78
 C      -2.266420    -3.419197    -0.672461     110.00
 O      -3.019207    -4.216825    -1.563695     238.33
 H      -2.378790    -4.516143    -2.212874      29.51
 H      -2.802045    -3.208709     0.327275      23.47
 H      -1.199164    -3.772779    -0.546270      24.67
 C       1.971026    -1.183929    -1.970894      68.97
 H       2.299320    -1.787189    -2.819053      17.97
 C       2.194660     0.037251     0.137750      78.06
 H       2.802312     0.659041     0.881639      14.88
 C       0.857530    -0.231302     0.480925      18.24
 O       0.103802     0.308519     1.582383     214.03
 C       0.703317     1.455278     2.233392      88.92
 H      -0.026253     1.563081     3.042929      23.46
 H       1.742213     1.163871     2.666207      22.28
 H       0.750003     2.410315     1.494199      21.53
 C       0.040600    -0.971874    -0.458755      20.28
 O      -1.270865    -1.138019    -0.046223     162.12
 C       0.714636    -1.547847    -1.600469      66.75
 H       0.173456    -2.281461    -2.365908      18.76
 C       2.717815    -0.290539    -1.181892      58.26
 C       4.139055     0.131252    -1.567718      91.65
 H       4.302288    -0.219541    -2.498786      25.93
 O       4.304338     1.591023    -1.614200     231.91
 H       4.697968     1.700651    -0.688332      24.28
 C       5.315190    -0.552733    -0.814127     101.14
 H       5.400018    -0.357577     0.222587      27.97
 O       5.241611    -1.943588    -1.101558     348.60
 H       5.159259    -2.254912    -1.997045      30.24
 C       6.722805    -0.182350    -1.377838      88.27
 O       7.347096     1.178266    -1.232823     261.50
 H       7.745809     1.338909    -0.370381      31.94
 H       6.612276    -0.354131    -2.519821      32.80
 H       7.320999    -1.010132    -0.867005      31.91
55
name= lig-ACN-Water-frame_194
 C      -3.959138     0.066961    -2.992770      41.06
 H      -4.312008    -0.834546    -3.493346      15.46
 C      -3.551349     1.471891    -1.023891      55.48
 H      -3.425283     1.451442     0.016790      21.44
 C      -3.579313     2.666540    -1.836746       4.53
 O      -3.689123     3.950340    -1.280051     227.37
 C      -4.235928     4.132235    -0.006551     133.27
 H      -3.652567     3.685172     0.718415      28.49
 H      -5.299818     3.909405     0.106886      27.57
 H      -4.299900     5.174100     0.093539      25.61
 C      -3.534331     2.478582    -3.248860      11.24
 O      -3.324663     3.468955    -4.104452     157.59
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 H      -3.321789     4.294074    -3.629559      21.68
 C      -3.900672     1.191575    -3.813363      56.96
 H      -3.990336     1.188248    -4.832524      32.22
 C      -3.699334     0.170806    -1.628145      23.08
 C      -3.623455    -1.164956    -0.742762      98.34
 H      -4.319605    -1.821719    -1.083076      26.79
 O      -3.960775    -1.033597     0.616634     267.43
 H      -3.263906    -0.401589     0.949304      24.79
 C      -2.266536    -1.836260    -0.998582      96.38
 H      -1.926960    -1.666269    -1.997650      25.31
 C      -2.276285    -3.322497    -0.675049     105.11
 O      -3.084909    -4.248755    -1.602645     182.98
 H      -2.493412    -4.505620    -2.416578      27.11
 H      -2.640864    -3.763436     0.332399      23.71
 H      -1.191453    -3.711028    -0.682201      23.48
 C       1.974945    -1.093002    -1.989489      49.16
 H       2.491858    -1.260608    -2.938878      20.68
 C       2.188147     0.143751     0.104966      75.02
 H       2.867773     0.655503     0.749804      20.20
 C       0.855002    -0.244788     0.481825      14.95
 O       0.198041     0.269944     1.535411     213.30
 C       0.700290     1.477957     2.203278      88.86
 H       0.034179     1.772992     3.058406      24.11
 H       1.829643     1.396773     2.647142      21.67
 H       0.684875     2.372679     1.465329      23.68
 C       0.069837    -0.999021    -0.408269      17.66
 O      -1.299602    -1.170351    -0.126024     193.10
 C       0.669444    -1.562091    -1.510002      68.95
 H      -0.087172    -2.213321    -2.171904      19.00
 C       2.774953    -0.316062    -1.089558      32.20
 C       4.153381     0.141527    -1.565308      83.10
 H       4.201597    -0.061192    -2.543810      23.88
 O       4.284813     1.621257    -1.605599     243.74
 H       4.493842     2.022272    -0.791833      28.60
 C       5.329061    -0.544561    -0.842723      96.72
 H       5.113257    -0.549146     0.226712      24.27
 O       5.209088    -1.979230    -1.115060     328.59
 H       5.107524    -1.900819    -2.090433      26.87
 C       6.781593    -0.123727    -1.375241     103.01
 O       7.325855     1.197988    -1.250097     262.88
 H       7.721308     1.188045    -0.371210      31.14
 H       6.854973    -0.378594    -2.512451      32.94
 H       7.609981    -0.829721    -0.922806      28.99
55
name= lig-ACN-Water-frame_195
 C      -3.970225     0.025430    -2.959885      59.67
 H      -4.154685    -1.027073    -3.336919      26.61
 C      -3.564072     1.473040    -0.983248      58.26
 H      -3.330466     1.642418     0.035480      20.71
 C      -3.659740     2.636238    -1.769316      -4.05
 O      -3.743681     3.959380    -1.360486     179.45
 C      -4.232549     4.173650     0.065798     117.94
 H      -3.624116     3.848267     0.743885      30.53
 H      -5.142561     3.569282     0.118246      28.86
 H      -4.214990     5.275094     0.164292      24.16
 C      -3.580515     2.427338    -3.207431      15.36
 O      -3.330661     3.491930    -4.118164     114.03
 H      -3.503275     4.403696    -3.735838      21.52
 C      -3.823088     1.181754    -3.776409      66.56
 H      -3.884137     1.081477    -4.805643      27.25
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 C      -3.734660     0.175687    -1.556067      19.45
 C      -3.663041    -1.132866    -0.816941      91.89
 H      -4.338867    -1.768331    -1.208656      25.10
 O      -3.961218    -0.980799     0.603414     285.97
 H      -3.295648    -0.772142     1.381659      19.74
 C      -2.282301    -1.875456    -1.006998      82.40
 H      -2.082269    -1.820406    -2.036579      27.09
 C      -2.264787    -3.425899    -0.692014     106.94
 O      -3.095921    -4.207027    -1.628312     195.99
 H      -2.565194    -4.107862    -2.497247      28.74
 H      -2.601109    -3.507583     0.392022      24.89
 H      -1.172170    -3.733527    -0.911290      23.65
 C       1.959179    -1.050335    -1.919546      20.40
 H       2.126134    -1.288747    -2.964192      21.30
 C       2.217996     0.201364     0.122398      68.61
 H       2.579441     0.894214     0.770662      16.33
 C       0.864492    -0.147530     0.434006      17.30
 O       0.249868     0.270306     1.613494     213.93
 C       0.700531     1.513048     2.162380      98.76
 H      -0.064916     1.722225     2.985147      22.44
 H       1.841491     1.323834     2.629804      20.76
 H       0.681229     2.282867     1.367529      24.68
 C       0.069104    -1.104974    -0.394884      12.59
 O      -1.317558    -1.184569    -0.128796     155.58
 C       0.687628    -1.523577    -1.590077      80.26
 H       0.197820    -2.194212    -2.416502      19.00
 C       2.779002    -0.324258    -1.080321      44.50
 C       4.155796     0.223070    -1.617972      85.74
 H       4.215464    -0.051859    -2.583671      25.14
 O       4.255473     1.680330    -1.587094     258.93
 H       4.546600     1.828864    -0.642666      23.28
 C       5.386587    -0.552579    -0.881855      92.34
 H       5.368336    -0.310906     0.216513      24.24
 O       5.163167    -1.989690    -1.165388     270.91
 H       5.375527    -2.281719    -2.110970      30.19
 C       6.837031    -0.156718    -1.371829      88.94
 O       7.271552     1.237380    -1.239467     252.28
 H       7.506625     1.468705    -0.242804      26.61
 H       6.729888    -0.338032    -2.500757      31.88
 H       7.543958    -0.953190    -0.816086      29.59
55
name= lig-ACN-Water-frame_196
 C      -3.941837     0.056110    -2.892421      83.54
 H      -3.978566    -1.001022    -3.366112      27.51
 C      -3.596896     1.458844    -0.917127      54.71
 H      -3.582837     1.499664     0.189002      19.89
 C      -3.714087     2.582060    -1.798320       4.02
 O      -3.781906     3.953786    -1.382319     211.52
 C      -4.172623     4.181213     0.049960     118.59
 H      -3.441320     3.959183     0.605603      30.53
 H      -5.110631     3.695283     0.330589      27.44
 H      -4.555893     5.280703     0.148217      24.02
 C      -3.674285     2.473236    -3.201287      -0.47
 O      -3.376239     3.508818    -4.072371      71.06
 H      -3.592841     4.445954    -3.638090      20.57
 C      -3.756568     1.137263    -3.757729      25.44
 H      -3.693255     1.107916    -4.844116      17.44
 C      -3.770931     0.185997    -1.518948       5.32
 C      -3.640787    -1.130228    -0.748884      90.42
 H      -4.361821    -1.690193    -1.156132      25.23
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 O      -4.051798    -0.996923     0.598486     272.74
 H      -3.187087    -0.680149     1.013373      22.60
 C      -2.250671    -1.920559    -1.049777      82.28
 H      -1.908861    -1.694966    -2.007241      27.36
 C      -2.238115    -3.472368    -0.724384     113.86
 O      -3.093383    -4.117810    -1.645941     249.48
 H      -2.657413    -4.219981    -2.486449      31.14
 H      -2.665984    -3.732771     0.271900      25.13
 H      -1.168567    -3.922124    -0.622887      25.39
 C       1.987976    -1.081595    -1.935751      22.09
 H       2.591379    -1.436113    -2.772683      19.37
 C       2.180776     0.217390     0.120063      53.91
 H       2.800414     0.871384     0.620412      18.69
 C       0.796163    -0.172943     0.401340      19.59
 O       0.247064     0.239680     1.658669     214.65
 C       0.701533     1.546878     2.154738      98.50
 H      -0.046999     1.881909     2.961752      23.39
 H       1.813093     1.516247     2.751496      21.65
 H       0.722529     2.297975     1.419693      26.55
 C       0.060066    -1.074782    -0.409810      17.88
 O      -1.295028    -1.216836    -0.095785     180.02
 C       0.667989    -1.478882    -1.645454      73.66
 H       0.092137    -2.087137    -2.372191      19.96
 C       2.812579    -0.187546    -1.115003      48.19
 C       4.187661     0.224986    -1.648972      86.66
 H       4.219365     0.056559    -2.692525      25.50
 O       4.233571     1.724484    -1.509880     222.20
 H       4.852256     1.985617    -0.701439      21.75
 C       5.385907    -0.534846    -0.992206      96.34
 H       5.298159    -0.528540     0.150603      25.85
 O       5.148679    -1.957148    -1.157987     300.33
 H       5.312680    -2.001759    -2.162123      29.10
 C       6.817865    -0.184000    -1.405950     100.09
 O       7.185036     1.240302    -1.216510     253.74
 H       7.476560     1.334059    -0.204768      26.11
 H       7.076521    -0.377953    -2.476062      32.75
 H       7.619523    -0.864970    -0.801690      30.26
55
name= lig-ACN-Water-frame_197
 C      -3.844616     0.078767    -2.890101      74.74
 H      -3.967173    -0.984014    -3.355703      33.40
 C      -3.721528     1.471429    -0.911591      50.58
 H      -3.686582     1.641271     0.226769      20.61
 C      -3.755677     2.627626    -1.754751       3.98
 O      -3.837955     3.906986    -1.348973     190.02
 C      -4.116774     4.194106    -0.016326     122.45
 H      -3.356273     4.143107     0.568399      31.98
 H      -4.808112     3.455987     0.364359      28.79
 H      -4.340650     5.356838    -0.099157      24.16
 C      -3.719316     2.453943    -3.217298       6.01
 O      -3.474481     3.542023    -3.992494       8.35
 H      -3.617305     4.395243    -3.446618      21.64
 C      -3.731714     1.194017    -3.756734      62.98
 H      -3.624622     0.980621    -4.875717      16.04
 C      -3.745026     0.159736    -1.484809     -45.79
 C      -3.659342    -1.212361    -0.757663      55.71
 H      -4.266427    -1.926849    -1.145998      25.87
 O      -4.081931    -1.056056     0.639556     190.24
 H      -3.609315    -0.524575     1.257103      25.71
 C      -2.174596    -1.887587    -0.946859      92.85
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 H      -1.980845    -1.809098    -1.992825      29.99
 C      -2.239916    -3.419575    -0.690421     111.13
 O      -3.115710    -4.080148    -1.737960     182.72
 H      -2.464027    -4.440536    -2.376278      28.70
 H      -2.698654    -3.565017     0.272667      26.41
 H      -1.205016    -3.874031    -0.809848      25.44
 C       2.101497    -1.104687    -1.968989      51.17
 H       2.490388    -1.656134    -2.821374      18.80
 C       2.126001     0.233794     0.029135      85.80
 H       2.568115     0.729024     0.880903      17.28
 C       0.854676    -0.180471     0.487487       4.86
 O       0.232945     0.219725     1.645281     210.11
 C       0.677889     1.567352     2.183273      77.91
 H      -0.142118     1.915304     2.876885      24.42
 H       1.790301     1.348412     2.714116      20.69
 H       0.770036     2.158627     1.335481      25.97
 C       0.045749    -0.932606    -0.497994      11.63
 O      -1.264761    -1.285588    -0.063292     177.60
 C       0.683819    -1.429600    -1.638086      68.50
 H       0.178674    -2.099962    -2.264176      23.58
 C       2.705585    -0.170798    -1.185425      29.78
 C       4.170171     0.323060    -1.636507      84.76
 H       4.193727     0.167782    -2.723018      26.46
 O       4.263468     1.741673    -1.420768     241.34
 H       5.006680     1.924543    -0.831398      24.30
 C       5.331646    -0.524776    -1.003065      84.34
 H       5.227833    -0.169359     0.096834      23.48
 O       5.166819    -1.930085    -1.212697     318.92
 H       4.846453    -2.138272    -2.105293      29.77
 C       6.823360    -0.154919    -1.433959      89.79
 O       7.088205     1.213321    -1.183500     282.77
 H       7.704777     1.294722    -0.428601      29.87
 H       6.865288    -0.462345    -2.477821      34.34
 H       7.478772    -0.844774    -0.709953      29.82
55
name= lig-ACN-Water-frame_198
 C      -3.731821     0.048997    -2.919848      60.73
 H      -3.737115    -0.996471    -3.373222      22.53
 C      -3.853589     1.440237    -0.922663      43.37
 H      -3.730142     1.660085     0.209542      17.08
 C      -3.810940     2.539686    -1.766344      14.19
 O      -3.858020     3.900512    -1.398047     213.93
 C      -4.042730     4.247062     0.030310     130.99
 H      -3.175445     4.183030     0.468671      30.54
 H      -4.832798     3.677703     0.510366      28.86
 H      -4.600624     5.286329     0.121549      25.08
 C      -3.700133     2.472707    -3.130573      -3.73
 O      -3.596323     3.616158    -3.936663      77.10
 H      -3.705598     4.507473    -3.556564      20.93
 C      -3.745623     1.184232    -3.745578      36.76
 H      -3.733469     1.218108    -4.919091      25.04
 C      -3.738234     0.139042    -1.490533     -25.59
 C      -3.602708    -1.206421    -0.701921      72.06
 H      -4.278652    -1.828879    -1.211175      22.88
 O      -4.131192    -1.170250     0.687302     217.82
 H      -3.334885    -0.780549     1.109039      25.78
 C      -2.229299    -1.865126    -0.900574      85.44
 H      -1.862486    -1.611480    -1.905299      25.20
 C      -2.299666    -3.387170    -0.696050     116.14
 O      -3.097809    -4.037936    -1.771721     216.86
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 H      -2.418154    -4.384355    -2.494428      24.32
 H      -2.616964    -3.686493     0.279421      25.87
 H      -1.251849    -3.753225    -0.734041      24.16
 C       2.000513    -1.148214    -2.002056      34.85
 H       2.420554    -1.465828    -2.948638      18.16
 C       2.111822     0.265434     0.035691      70.96
 H       2.853172     1.016478     0.479441      14.09
 C       0.825257    -0.174884     0.415210      13.68
 O       0.236529     0.233454     1.649743     222.65
 C       0.653815     1.477043     2.161586      93.13
 H      -0.177593     1.812964     2.806545      23.99
 H       1.602616     1.402884     2.932795      21.35
 H       0.900405     2.228053     1.422005      24.68
 C       0.056641    -0.848537    -0.503351      19.97
 O      -1.162722    -1.296476    -0.014366     180.82
 C       0.752693    -1.436668    -1.651385      75.37
 H       0.224336    -2.099222    -2.236988      22.19
 C       2.751608    -0.156360    -1.223160      38.87
 C       4.080039     0.379975    -1.652728      84.89
 H       4.210867     0.232203    -2.750857      21.78
 O       4.322959     1.784242    -1.343318     235.65
 H       4.942402     1.838897    -0.619065      21.45
 C       5.283643    -0.463629    -0.976646     102.31
 H       5.251070    -0.525775     0.167693      24.15
 O       5.138072    -1.923041    -1.214461     317.52
 H       5.095582    -1.983786    -2.216907      28.79
 C       6.683278    -0.188745    -1.401379     102.42
 O       7.057422     1.254957    -1.188903     306.25
 H       7.535349     1.340798    -0.368642      33.76
 H       6.830658    -0.262053    -2.457898      33.61
 H       7.462387    -0.930398    -0.976030      30.13
55
name= lig-ACN-Water-frame_199
 C      -3.654768     0.015698    -2.933354      57.90
 H      -3.459853    -0.948473    -3.420185      22.92
 C      -3.910008     1.369046    -0.888312      61.22
 H      -4.055413     1.303710     0.236240      19.46
 C      -3.873110     2.590031    -1.719244     -11.93
 O      -3.902295     3.926680    -1.355445     211.87
 C      -4.016235     4.275117     0.057086     118.94
 H      -3.086449     4.229109     0.506967      28.45
 H      -4.591519     3.542101     0.601458      26.19
 H      -4.220220     5.388475    -0.012769      23.59
 C      -3.710415     2.509146    -3.172188       4.85
 O      -3.719282     3.618137    -3.929196     135.33
 H      -3.750532     4.383316    -3.347989      22.04
 C      -3.740244     1.205680    -3.729177      26.27
 H      -3.816635     1.092059    -4.881591      25.07
 C      -3.739379     0.123864    -1.509864      17.17
 C      -3.636216    -1.147911    -0.669500      93.28
 H      -4.233266    -1.908636    -1.161952      24.81
 O      -4.071714    -1.245129     0.689417     207.43
 H      -3.437221    -1.088995     1.481194      21.88
 C      -2.230067    -1.832322    -0.881602      65.69
 H      -1.996031    -1.670262    -1.996555      25.33
 C      -2.292083    -3.414925    -0.721271     115.83
 O      -3.071041    -3.993245    -1.753399     215.75
 H      -2.523985    -4.006370    -2.617950      26.91
 H      -2.881911    -3.641842     0.136478      25.50
 H      -1.289500    -3.818065    -0.690177      26.03
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 C       2.037217    -1.026190    -2.045387      70.75
 H       2.517916    -1.428355    -2.931673      20.36
 C       2.195969     0.311531    -0.039196      73.96
 H       2.541858     1.210296     0.595627      12.44
 C       0.877624    -0.016832     0.362389      22.98
 O       0.274703     0.182145     1.562257     226.59
 C       0.643287     1.454416     2.244288      95.45
 H      -0.226760     1.871233     2.718573      23.73
 H       1.537901     1.207709     2.962242      22.47
 H       0.954552     2.159902     1.408693      25.00
 C       0.101355    -0.968342    -0.499128      13.61
 O      -1.152313    -1.305162     0.044876     173.07
 C       0.614873    -1.503436    -1.644513      97.37
 H       0.048453    -2.163003    -2.265760      20.75
 C       2.698467    -0.169867    -1.210397      32.74
 C       4.134809     0.366535    -1.604200      69.08
 H       4.179077     0.388831    -2.749127      21.14
 O       4.336049     1.823350    -1.305936     214.87
 H       4.680892     1.967703    -0.342900      21.68
 C       5.180479    -0.534581    -0.924125      95.22
 H       4.951753    -0.259031     0.157045      24.36
 O       5.053916    -1.901025    -1.233197     333.76
 H       5.465742    -2.100462    -2.149664      29.98
 C       6.618111    -0.076168    -1.432087      99.42
 O       7.061625     1.267362    -1.186976     310.80
 H       7.380222     1.221769    -0.224338      30.70
 H       6.519952    -0.314688    -2.471646      34.09
 H       7.317293    -0.767796    -0.912515      29.08
55
name= lig-ACN-Water-frame_200
 C      -3.611033     0.057477    -2.926434      81.31
 H      -3.448193    -0.902200    -3.353075      26.99
 C      -3.951330     1.429846    -0.925808      60.81
 H      -4.132714     1.577649     0.130046      22.13
 C      -3.887608     2.578027    -1.677968       0.08
 O      -3.975691     3.928135    -1.274683     199.13
 C      -3.918501     4.295459     0.079753     146.27
 H      -2.935532     4.091855     0.445897      25.95
 H      -4.719050     3.819842     0.654475      27.52
 H      -4.297817     5.302851     0.196574      25.59
 C      -3.811060     2.442752    -3.089637     -10.81
 O      -3.836240     3.587726    -3.949315     104.78
 H      -3.697142     4.545498    -3.596650      18.67
 C      -3.710752     1.187179    -3.725874      97.89
 H      -3.612855     1.123102    -4.831468      27.48
 C      -3.752908     0.126876    -1.498396     -45.26
 C      -3.589535    -1.232377    -0.690984      46.60
 H      -4.328066    -1.889085    -1.214962      22.16
 O      -4.037417    -1.261062     0.717943     192.54
 H      -3.254500    -0.762959     1.171101      24.37
 C      -2.151633    -1.864379    -0.859469      77.32
 H      -1.749680    -1.562848    -1.926576      24.54
 C      -2.288248    -3.380255    -0.666392     113.80
 O      -3.088990    -3.966769    -1.800228     228.95
 H      -2.498848    -4.022118    -2.549934      29.06
 H      -2.756177    -3.570401     0.299849      25.29
 H      -1.341579    -3.863414    -0.600857      26.43
 C       1.893410    -1.009181    -2.065095      19.96
 H       2.340709    -1.438080    -2.963227      23.28
 C       2.144031     0.449656    -0.032455      75.61
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 H       2.844921     1.005950     0.645387      17.63
 C       0.863655    -0.070734     0.255381      16.87
 O       0.318292     0.208965     1.512824     210.49
 C       0.647592     1.393773     2.292701     103.47
 H      -0.268129     1.685433     2.769597      24.79
 H       1.389918     1.174126     3.102751      23.65
 H       1.133591     2.254576     1.653910      23.32
 C       0.141199    -1.061453    -0.418950       7.45
 O      -1.210205    -1.316471     0.059650     169.81
 C       0.699201    -1.484716    -1.706921      73.38
 H       0.216302    -2.260526    -2.364020      20.19
 C       2.731687    -0.073868    -1.271116      32.83
 C       4.091530     0.396836    -1.588759      81.95
 H       4.398504     0.202627    -2.726388      21.47
 O       4.297105     1.803761    -1.290762     207.29
 H       4.586993     1.883122    -0.277160      21.24
 C       5.169429    -0.470240    -0.909724     106.60
 H       5.177857    -0.565436     0.191943      26.35
 O       4.965138    -1.919196    -1.199694     293.72
 H       5.017331    -2.014063    -2.256000      26.93
 C       6.559910    -0.047839    -1.405870     113.96
 O       7.074837     1.280379    -1.169997     288.93
 H       7.701269     1.344684    -0.321914      27.53
 H       6.584690    -0.016865    -2.482777      34.35
 H       7.275045    -0.786616    -1.104807      32.09
55
name= lig-ACN-Water-frame_201
 C      -3.614845     0.039606    -2.858022      82.91
 H      -3.439481    -0.895526    -3.344312      26.10
 C      -3.964147     1.432647    -0.862368      64.41
 H      -3.921319     1.523598     0.176988      20.42
 C      -3.927281     2.620649    -1.713279      16.68
 O      -4.067032     3.907757    -1.267160     217.40
 C      -3.884039     4.292127     0.180836     114.34
 H      -2.873999     3.947759     0.542962      28.59
 H      -4.558955     3.758864     0.851498      28.40
 H      -3.809369     5.304868     0.102520      26.83
 C      -3.913859     2.510050    -3.118902       6.33
 O      -3.952237     3.502843    -3.980022     154.97
 H      -3.917972     4.371617    -3.375527      20.34
 C      -3.660215     1.218748    -3.692533      30.63
 H      -3.456995     1.305373    -4.731258      18.25
 C      -3.744497     0.139318    -1.447318      -7.80
 C      -3.557691    -1.243963    -0.725894      74.42
 H      -4.177758    -2.092880    -1.239026      23.36
 O      -3.951397    -1.204380     0.676133     204.66
 H      -3.468431    -0.617462     1.268081      25.19
 C      -2.127338    -1.897747    -0.895275      72.10
 H      -1.736017    -1.812333    -2.020417      24.73
 C      -2.272128    -3.412322    -0.659951     113.42
 O      -3.102212    -3.922181    -1.783333     186.46
 H      -2.512578    -4.362578    -2.420375      27.15
 H      -2.890088    -3.674276     0.239271      25.87
 H      -1.326651    -3.878481    -0.662016      27.62
 C       1.983028    -0.907370    -2.091365      30.84
 H       2.379004    -1.176577    -3.082465      19.71
 C       2.065596     0.430774    -0.138150      80.80
 H       2.600473     0.997938     0.577836      18.92
 C       0.874468    -0.120961     0.344320      11.66
 O       0.296970     0.250341     1.495968     240.07
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 C       0.677121     1.316583     2.367882     106.03
 H      -0.249713     1.714004     2.818659      24.64
 H       1.317709     0.942749     3.119746      25.22
 H       1.132997     2.212004     1.761028      23.53
 C       0.088891    -1.096046    -0.460165      11.37
 O      -1.165212    -1.308797     0.077586     162.36
 C       0.682055    -1.498731    -1.625066      75.87
 H       0.171024    -2.281353    -2.322875      20.24
 C       2.603003     0.026172    -1.340052      41.47
 C       4.078197     0.394328    -1.605727      80.66
 H       4.169306     0.351424    -2.831430      23.27
 O       4.244400     1.786779    -1.293621     194.11
 H       4.832034     1.897339    -0.493887      24.12
 C       5.198726    -0.475465    -0.876975      89.87
 H       5.072754    -0.235016     0.189702      26.25
 O       4.899733    -1.886584    -1.190560     342.37
 H       4.640935    -1.989764    -2.141001      28.35
 C       6.618116    -0.076394    -1.458672     105.07
 O       7.121638     1.329280    -1.104531     282.37
 H       7.686832     1.175508    -0.269250      26.40
 H       6.451613    -0.210996    -2.532545      34.54
 H       7.271948    -0.801842    -1.126825      32.33
55
name= lig-ACN-Water-frame_202
 C      -3.630524     0.078951    -2.852541      84.46
 H      -3.387931    -0.888967    -3.312281      27.32
 C      -3.884951     1.420239    -0.834847      61.05
 H      -3.896812     1.534412     0.204357      19.66
 C      -4.041775     2.572382    -1.642240      13.25
 O      -4.161844     3.933713    -1.199712     222.37
 C      -3.803133     4.221974     0.161357     126.13
 H      -2.848980     3.622404     0.428125      24.96
 H      -4.652027     4.049815     0.817557      27.80
 H      -3.742976     5.211492     0.239632      26.17
 C      -3.939260     2.427766    -3.107969      13.40
 O      -4.082897     3.551816    -4.027583     132.93
 H      -4.161645     4.510347    -3.656409      22.08
 C      -3.641716     1.210832    -3.621598      75.73
 H      -3.504282     1.018386    -4.618344      21.28
 C      -3.713331     0.137032    -1.443025       4.24
 C      -3.492163    -1.155937    -0.702403      75.50
 H      -4.370428    -1.800603    -1.202759      20.23
 O      -3.917710    -1.172714     0.622889     269.35
 H      -3.163684    -0.830338     1.119399      24.96
 C      -2.139541    -1.922728    -0.882422      77.86
 H      -1.822529    -1.711233    -2.002155      23.53
 C      -2.272721    -3.486490    -0.689598     116.33
 O      -3.122421    -3.925883    -1.741906     219.40
 H      -2.540417    -4.325661    -2.512576      24.69
 H      -2.726014    -3.621446     0.353235      25.32
 H      -1.317448    -3.978175    -0.645433      25.47
 C       1.909400    -0.921905    -2.162300      41.37
 H       2.368592    -1.309787    -3.095261      21.59
 C       2.027939     0.441598    -0.118174      52.61
 H       2.347139     1.323648     0.319500      17.17
 C       0.819732    -0.169495     0.405284      17.71
 O       0.151952     0.244006     1.551745     215.04
 C       0.734054     1.280889     2.452705     109.13
 H      -0.164650     1.726111     2.954091      23.98
 H       1.379632     0.891917     3.126515      26.46
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 H       1.328898     2.041221     1.858057      23.17
 C       0.138743    -0.988773    -0.437656      15.72
 O      -1.146574    -1.356664     0.020946     180.50
 C       0.750249    -1.502880    -1.646304      63.19
 H       0.144200    -2.229502    -2.327510      17.65
 C       2.609189     0.063522    -1.377445      31.41
 C       4.048609     0.439603    -1.662248      77.00
 H       4.354865     0.240797    -2.850700      20.62
 O       4.237880     1.830044    -1.303704     255.20
 H       4.811529     1.900336    -0.560053      22.74
 C       5.126394    -0.452782    -0.967563      96.27
 H       5.126352    -0.336950     0.114692      25.37
 O       4.865265    -1.820503    -1.123415     354.92
 H       4.978800    -2.040754    -2.073511      28.72
 C       6.675597    -0.068312    -1.461243     105.64
 O       7.150295     1.257480    -1.066393     341.27
 H       7.512430     1.250821    -0.173583      30.90
 H       6.790665    -0.001348    -2.563949      32.61
 H       7.350026    -0.721819    -1.078336      31.46
55
name= lig-ACN-Water-frame_203
 C      -3.597529     0.041668    -2.820951      60.00
 H      -3.465508    -0.983665    -3.289880      24.48
 C      -3.819502     1.443091    -0.821936      57.57
 H      -3.877103     1.456413     0.269327      19.78
 C      -4.117728     2.597560    -1.646037       6.61
 O      -4.257665     3.874837    -1.182397     287.94
 C      -3.778234     4.160146     0.145452     105.39
 H      -2.870270     3.454633     0.479430      25.56
 H      -4.505823     3.882682     0.892613      24.61
 H      -3.412828     5.091876     0.112226      26.39
 C      -3.986327     2.545561    -3.052093     -14.49
 O      -4.214058     3.545001    -4.014877     271.71
 H      -3.964504     4.369730    -3.545580      28.38
 C      -3.687701     1.198020    -3.678406      22.89
 H      -3.640567     1.284820    -4.737846      19.91
 C      -3.610791     0.192589    -1.434230      27.93
 C      -3.504583    -1.173861    -0.714814      77.98
 H      -4.156487    -1.990921    -1.340925      21.79
 O      -3.905306    -1.147501     0.672438     291.55
 H      -3.249705    -0.784543     1.352897      21.84
 C      -2.121028    -1.933819    -0.930577      78.58
 H      -1.746977    -1.796082    -2.018678      22.77
 C      -2.254360    -3.441217    -0.682489     106.52
 O      -3.178513    -4.021419    -1.722063     185.61
 H      -2.620049    -3.986962    -2.570701      28.29
 H      -2.763669    -3.805546     0.287707      24.61
 H      -1.279313    -3.935109    -0.814376      25.06
 C       1.917457    -0.935637    -2.154254      22.77
 H       2.389772    -1.420473    -3.032703      24.27
 C       2.026389     0.510665    -0.099912      63.50
 H       2.620198     1.311217     0.350085      17.25
 C       0.802031    -0.068901     0.428440      -3.73
 O       0.042567     0.270350     1.648315     194.48
 C       0.786336     1.217000     2.493536     120.84
 H       0.014572     1.783939     3.136067      24.35
 H       1.411605     0.760308     3.107447      27.65
 H       1.232059     1.984502     1.901291      25.66
 C       0.118628    -1.046149    -0.478893       7.01
 O      -1.125472    -1.419883    -0.038382     185.11
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 C       0.708282    -1.458104    -1.670866      59.03
 H       0.201256    -2.283127    -2.242759      19.30
 C       2.593625    -0.009890    -1.355290      31.19
 C       4.039069     0.511858    -1.722540      68.93
 H       4.109885     0.533383    -2.978660      20.25
 O       4.270240     1.890936    -1.348341     238.23
 H       4.593175     1.971644    -0.388215      22.56
 C       5.184063    -0.356317    -1.039697      99.43
 H       5.079230    -0.092160     0.008471      25.53
 O       4.845858    -1.819412    -1.109300     280.73
 H       5.243348    -2.237642    -1.950250      28.48
 C       6.657279    -0.070011    -1.418197     109.15
 O       7.163660     1.205571    -1.044239     339.70
 H       7.544182     1.076092    -0.161024      29.19
 H       6.688372    -0.214183    -2.530259      31.72
 H       7.130171    -0.892634    -1.061286      32.49
55
name= lig-ACN-Water-frame_204
 C      -3.555312     0.123116    -2.891409      51.25
 H      -3.466156    -0.887222    -3.423706      25.42
 C      -3.806294     1.472086    -0.857752      47.64
 H      -3.848120     1.619570     0.274857      18.59
 C      -4.064781     2.583134    -1.679050      19.24
 O      -4.357980     3.843007    -1.144751     219.70
 C      -3.744009     4.085773     0.179315     118.41
 H      -2.784531     3.348491     0.238383      22.55
 H      -4.459488     4.067879     0.971701      25.77
 H      -3.481696     5.113783     0.133514      24.66
 C      -4.033122     2.452691    -3.122436      26.60
 O      -4.317011     3.553289    -3.911793     249.74
 H      -4.083373     4.427839    -3.635789      22.33
 C      -3.807544     1.280268    -3.655159     118.11
 H      -3.719145     1.141574    -4.738374      25.88
 C      -3.519518     0.171076    -1.446856     -42.51
 C      -3.459166    -1.197524    -0.680540      61.50
 H      -4.418139    -1.841193    -1.084351      19.47
 O      -3.955992    -1.181551     0.684940     208.56
 H      -3.283237    -0.596869     1.181042      23.64
 C      -2.136135    -1.944281    -0.977911      78.40
 H      -1.884701    -1.783160    -2.062152      25.13
 C      -2.283510    -3.473646    -0.757506     109.08
 O      -3.197779    -4.105424    -1.695039     214.18
 H      -2.846685    -4.062361    -2.565376      30.66
 H      -2.652607    -3.554249     0.345273      24.07
 H      -1.236639    -3.903744    -0.766597      24.93
 C       1.982472    -0.962308    -2.059421      36.06
 H       2.490126    -1.242881    -3.001268      16.37
 C       1.992637     0.491874    -0.086678      74.18
 H       2.580429     1.078227     0.731968      16.54
 C       0.728876     0.013648     0.357951      12.89
 O       0.104199     0.300408     1.609447     225.04
 C       0.787474     1.199140     2.531010     119.16
 H       0.035536     1.580741     3.296192      23.49
 H       1.626424     0.739993     2.933988      25.81
 H       1.185491     1.943991     1.961118      25.64
 C       0.126874    -1.002498    -0.427173       9.39
 O      -1.112346    -1.474837    -0.022623     173.09
 C       0.648099    -1.453358    -1.687628      74.45
 H       0.177059    -2.224650    -2.261039      22.83
 C       2.630656     0.020825    -1.276880      36.68
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 C       4.017607     0.550636    -1.745547      70.01
 H       4.012318     0.575216    -3.015254      20.62
 O       4.300026     1.959275    -1.410153     215.75
 H       4.641380     2.051043    -0.412162      19.97
 C       5.116033    -0.323782    -1.057935      89.83
 H       5.038835    -0.055385    -0.007942      23.89
 O       4.883574    -1.772333    -1.092484     297.81
 H       4.969371    -1.990892    -2.121548      29.69
 C       6.605447    -0.170232    -1.449743     109.67
 O       7.186800     1.158281    -1.068961     313.10
 H       7.590634     1.169678    -0.156082      27.16
 H       6.763493    -0.216949    -2.551645      32.35
 H       7.184945    -0.835648    -0.924256      32.32
55
name= lig-ACN-Water-frame_205
 C      -3.524054     0.152248    -2.887198      65.98
 H      -3.239288    -0.798636    -3.430948      23.89
 C      -3.772439     1.390640    -0.927251      66.04
 H      -3.866194     1.492328     0.221827      18.45
 C      -4.006773     2.575692    -1.674131      16.41
 O      -4.415354     3.793327    -1.085362     277.37
 C      -3.739774     4.096364     0.154868     112.08
 H      -2.700632     3.458305     0.425673      22.07
 H      -4.340666     3.735626     0.961558      26.89
 H      -3.429413     5.175126     0.218192      24.02
 C      -4.124786     2.544582    -3.072323      -9.39
 O      -4.429839     3.599680    -3.865716     270.73
 H      -4.108147     4.368210    -3.361843      29.09
 C      -3.875497     1.200734    -3.738208      18.31
 H      -3.984275     1.135327    -4.875645      20.00
 C      -3.512793     0.188596    -1.484364      38.40
 C      -3.502778    -1.161150    -0.697087      79.29
 H      -4.208730    -1.837339    -1.447148      23.05
 O      -3.982604    -1.203701     0.653070     216.37
 H      -3.360634    -0.839764     1.401226      21.42
 C      -2.173296    -1.972444    -0.983116      84.67
 H      -1.804241    -1.605172    -1.914768      25.43
 C      -2.283209    -3.503561    -0.797987     105.41
 O      -3.215261    -4.179215    -1.665593     203.12
 H      -2.664866    -4.405081    -2.470076      28.20
 H      -2.765387    -3.723449     0.222623      23.99
 H      -1.287793    -4.103276    -0.862073      23.63
 C       1.980412    -0.947108    -1.961612      70.79
 H       2.348720    -1.320290    -2.918618      14.71
 C       1.995317     0.457889     0.002778      73.13
 H       2.548705     1.336261     0.645929      14.80
 C       0.709624     0.016323     0.301751      24.45
 O       0.179438     0.314931     1.516883     216.65
 C       0.814399     1.224625     2.496079     111.30
 H       0.055001     1.178645     3.287954      23.39
 H       1.718640     0.788904     3.005932      22.35
 H       0.911809     2.198085     2.247201      25.30
 C       0.048349    -0.965608    -0.499562      12.02
 O      -1.149095    -1.522383     0.033318     169.82
 C       0.757437    -1.411569    -1.617493      51.88
 H       0.246235    -2.030087    -2.262004      21.35
 C       2.632040     0.091697    -1.231068      49.37
 C       3.998907     0.584145    -1.682864      68.38
 H       4.172947     0.279047    -2.909405      21.82
 O       4.314902     1.993857    -1.483779     226.11
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 H       4.986630     2.011355    -0.734760      21.55
 C       5.081739    -0.339504    -1.017676      86.39
 H       5.027240    -0.148164     0.066079      25.10
 O       4.895863    -1.721179    -1.127160     364.00
 H       4.691072    -2.056149    -2.037441      27.99
 C       6.628584    -0.148316    -1.454388      87.73
 O       7.196012     1.109031    -1.187557     347.16
 H       7.502654     1.019142    -0.205775      28.99
 H       6.717682    -0.397536    -2.529491      32.76
 H       7.048764    -1.045663    -1.030355      33.47
55
name= lig-ACN-Water-frame_206
 C      -3.509135     0.076688    -2.977724      52.69
 H      -3.239038    -0.880643    -3.444014      20.33
 C      -3.761737     1.424606    -0.870974      43.16
 H      -3.841007     1.369840     0.260026      16.99
 C      -4.034174     2.570890    -1.656891      29.61
 O      -4.390117     3.734967    -1.037839     227.35
 C      -3.734295     4.102490     0.211970     105.83
 H      -2.598304     3.646726     0.049411      18.99
 H      -4.311831     3.832698     1.108240      23.63
 H      -3.789723     5.275413     0.133985      21.01
 C      -4.163899     2.478124    -3.114500      -0.20
 O      -4.554531     3.652058    -3.823329     263.18
 H      -4.109759     4.550655    -3.585654      22.98
 C      -3.941985     1.282965    -3.707709      55.35
 H      -4.047837     1.237125    -4.842887      24.01
 C      -3.524018     0.149988    -1.548422     -18.33
 C      -3.499772    -1.192512    -0.816739      69.28
 H      -4.400485    -1.916787    -1.212254      19.84
 O      -4.035926    -1.230768     0.579552     193.00
 H      -3.288837    -0.822238     1.143013      21.91
 C      -2.162477    -1.956865    -0.920914      97.51
 H      -1.821684    -1.952331    -1.908881      24.61
 C      -2.307606    -3.563695    -0.744389      96.57
 O      -3.213719    -4.244075    -1.719855     177.80
 H      -2.654757    -4.671667    -2.484930      26.24
 H      -2.572190    -3.784824     0.327436      24.50
 H      -1.169457    -3.838054    -0.922697      21.96
 C       2.047826    -0.849649    -1.956064      46.38
 H       2.605613    -1.248880    -2.800419      12.32
 C       2.063752     0.516452    -0.020526      65.19
 H       2.444026     1.483063     0.640968      12.39
 C       0.772017    -0.017695     0.320900      23.58
 O       0.159079     0.353268     1.501437     212.10
 C       0.761826     1.209042     2.501519     114.74
 H       0.211043     1.038457     3.387450      24.39
 H       1.928937     1.031104     2.526925      21.68
 H       0.673726     2.185962     2.123103      24.90
 C      -0.028104    -0.933451    -0.474484      17.36
 O      -1.176873    -1.538435     0.047844     212.87
 C       0.728503    -1.455208    -1.568512      94.90
 H       0.436678    -2.242845    -2.191796      18.03
 C       2.635385     0.142413    -1.190023      44.60
 C       4.058203     0.536237    -1.630875      61.81
 H       3.986029     0.414181    -2.894121      18.39
 O       4.339846     1.988386    -1.555857     253.16
 H       5.064896     2.143442    -0.978370      24.85
 C       5.180873    -0.307925    -0.931426     109.18
 H       5.135766    -0.080745     0.156332      24.92
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 O       4.818819    -1.761207    -1.141116     372.67
 H       5.091791    -1.939335    -2.065571      29.25
 C       6.543967    -0.197755    -1.497205     120.01
 O       7.249860     1.099173    -1.276799     202.36
 H       7.620925     1.161473    -0.307632      29.55
 H       6.508926    -0.287343    -2.589825      35.73
 H       7.264178    -0.839598    -0.956945      30.73
55
name= lig-ACN-Water-frame_207
 C      -3.592461     0.132627    -3.044917      70.56
 H      -3.513536    -0.745092    -3.623854      20.31
 C      -3.749327     1.336748    -0.909675      58.74
 H      -3.735382     1.529017     0.157773      18.22
 C      -4.099640     2.500973    -1.617246       9.37
 O      -4.362652     3.731358    -1.014216     274.95
 C      -3.730027     4.154103     0.204139     106.31
 H      -2.519087     4.003104     0.424552      23.05
 H      -4.173262     3.617723     1.095980      24.33
 H      -3.857861     5.370669     0.305865      22.79
 C      -4.191068     2.552158    -3.031649      -2.25
 O      -4.672918     3.609845    -3.807051     286.71
 H      -4.206906     4.462651    -3.390018      22.81
 C      -3.928582     1.264807    -3.719544      41.23
 H      -3.938542     1.257245    -4.833874      24.61
 C      -3.554566     0.135330    -1.599833      10.60
 C      -3.526798    -1.285190    -0.844288      75.03
 H      -4.171271    -1.929382    -1.659636      22.56
 O      -4.048349    -1.206474     0.471363     217.20
 H      -3.431421    -0.893913     1.154208      21.53
 C      -2.195061    -2.093990    -0.943385      85.60
 H      -1.813963    -1.815106    -1.876692      24.64
 C      -2.289631    -3.586293    -0.702825     111.42
 O      -3.151456    -4.260018    -1.734263     182.38
 H      -2.534853    -4.387699    -2.472060      28.25
 H      -2.709385    -3.938221     0.236473      24.73
 H      -1.255132    -4.170723    -0.838407      22.34
 C       1.969583    -0.861652    -1.950769      15.59
 H       2.462391    -1.325681    -2.799271      18.97
 C       1.995220     0.631190    -0.005027      53.45
 H       2.593153     1.379375     0.720749      17.18
 C       0.771174    -0.000025     0.405706      12.77
 O       0.041396     0.355647     1.552391     218.18
 C       0.741754     1.235312     2.447345     111.12
 H       0.523486     1.011515     3.440244      25.71
 H       1.928095     1.017060     2.471561      21.71
 H       0.462318     2.313833     2.320031      23.62
 C       0.125349    -0.965259    -0.438636      -2.03
 O      -1.185894    -1.484851     0.043282     150.76
 C       0.794850    -1.440952    -1.594179      44.74
 H       0.345418    -2.330901    -2.022359      16.42
 C       2.734944     0.145887    -1.207831      55.03
 C       4.129832     0.559117    -1.630725      55.11
 H       4.370741     0.051803    -2.772060      18.75
 O       4.364699     1.984188    -1.625991     283.37
 H       4.876078     2.174054    -0.752692      21.38
 C       5.155003    -0.379782    -0.885014     120.29
 H       5.242154    -0.240930     0.232924      23.00
 O       4.763245    -1.739813    -1.076057     340.45
 H       4.942547    -2.052702    -2.005965      26.22
 C       6.624776    -0.172177    -1.527642      96.95
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 O       7.272997     1.119867    -1.331109     241.71
 H       7.493498     1.119476    -0.378076      33.64
 H       6.499888    -0.327677    -2.598499      37.46
 H       7.132721    -1.189318    -1.284527      33.65
55
name= lig-ACN-Water-frame_208
 C      -3.702621     0.136773    -3.013862      55.50
 H      -3.525098    -0.744740    -3.555431      32.27
 C      -3.744935     1.274627    -0.939803      55.48
 H      -3.564066     1.128346     0.074520      22.48
 C      -4.113648     2.517184    -1.584556      18.24
 O      -4.320661     3.767203    -1.011137     223.61
 C      -3.722362     4.199072     0.254544      93.41
 H      -2.567533     3.994617     0.071365      24.37
 H      -4.220008     3.613143     1.145514      24.96
 H      -4.106895     5.395148     0.330105      23.26
 C      -4.250293     2.502649    -3.033001      13.12
 O      -4.732565     3.545074    -3.752490     182.51
 H      -4.553815     4.517105    -3.364004      22.49
 C      -3.916637     1.399260    -3.768585      56.38
 H      -3.987420     1.457208    -4.839107      16.04
 C      -3.571125     0.020099    -1.648409       5.01
 C      -3.494138    -1.313932    -0.939692      60.05
 H      -4.331884    -2.062171    -1.327585      19.43
 O      -4.095500    -1.204125     0.390041     155.60
 H      -3.362860    -0.911809     0.977123      26.20
 C      -2.093919    -2.087473    -0.981144      69.18
 H      -1.792663    -2.127729    -2.004205      25.95
 C      -2.276253    -3.696359    -0.690593     110.00
 O      -3.052897    -4.240732    -1.735367     214.59
 H      -2.669021    -4.160528    -2.600320      28.45
 H      -2.879911    -3.689274     0.192057      25.51
 H      -1.207244    -4.113770    -0.438998      24.54
 C       2.065885    -0.867143    -1.984789      38.12
 H       2.485152    -1.192637    -2.936652      17.27
 C       1.968035     0.626511    -0.041122      63.02
 H       2.473183     1.422665     0.562320      17.00
 C       0.731684     0.061172     0.424255      -2.23
 O      -0.021095     0.361291     1.592360     191.89
 C       0.731895     1.266004     2.504810      89.70
 H       0.402031     0.928320     3.444083      23.36
 H       1.903814     1.171383     2.259729      21.03
 H       0.448448     2.404845     2.271134      22.17
 C       0.154112    -1.054341    -0.334145       8.70
 O      -1.130921    -1.413903     0.000923     150.05
 C       0.776036    -1.430920    -1.521964      61.72
 H       0.323872    -2.075252    -2.351959      20.33
 C       2.616519     0.120580    -1.208004      23.64
 C       4.159023     0.511994    -1.616575      58.33
 H       4.184907     0.357503    -2.872215      18.99
 O       4.409462     1.953927    -1.644924     274.69
 H       4.523911     2.280629    -0.640547      21.82
 C       5.238956    -0.391076    -0.894018      72.71
 H       5.195745    -0.111825     0.210326      21.89
 O       4.727839    -1.750381    -0.965198     355.72
 H       4.507576    -1.942286    -1.942573      24.83
 C       6.636056    -0.193071    -1.582102     108.63
 O       7.247016     1.074773    -1.294196     232.04
 H       7.443069     1.175356    -0.360866      33.94
 H       6.491604    -0.129202    -2.656204      33.81
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 H       7.496188    -0.894498    -1.191842      27.84
55
name= lig-ACN-Water-frame_209
 C      -3.733938     0.112742    -3.177342      71.45
 H      -3.573970    -0.756194    -3.779327      29.18
 C      -3.734896     1.261771    -0.907498      59.55
 H      -3.673754     1.407148     0.117303      18.05
 C      -4.053610     2.481512    -1.557663      10.14
 O      -4.313299     3.788394    -1.032516     241.99
 C      -3.744158     4.183033     0.233326     105.50
 H      -2.572195     4.212280     0.328348      24.56
 H      -4.094740     3.594564     1.198987      24.50
 H      -3.954928     5.450574     0.342743      23.21
 C      -4.291378     2.480162    -2.976488      14.23
 O      -4.802894     3.563077    -3.716409     208.86
 H      -4.336245     4.395071    -3.281377      23.36
 C      -3.928609     1.341461    -3.727326      55.12
 H      -3.964699     1.401225    -4.777562      17.70
 C      -3.629357     0.054080    -1.697821      -2.15
 C      -3.457460    -1.368214    -0.999062      65.51
 H      -4.004513    -2.107918    -1.706946      21.66
 O      -4.076464    -1.219919     0.353774     117.46
 H      -3.493967    -0.768777     1.089277      19.55
 C      -1.993793    -2.100168    -0.990204      86.83
 H      -1.499587    -1.924391    -1.947476      23.28
 C      -2.257624    -3.592254    -0.600313     107.85
 O      -2.990601    -4.249348    -1.741178     186.18
 H      -2.313459    -4.332513    -2.515019      25.38
 H      -2.859938    -3.815634     0.248478      24.78
 H      -1.335879    -4.251462    -0.467571      24.10
 C       2.021588    -0.906670    -1.955219      32.34
 H       2.493102    -1.182254    -2.898987      16.53
 C       1.915324     0.587619    -0.040835      70.21
 H       2.243373     1.492264     0.347747      16.89
 C       0.684281     0.021951     0.408227      16.99
 O       0.053171     0.414149     1.574025     217.90
 C       0.668195     1.273958     2.560140      93.33
 H       0.377607     1.081505     3.626090      22.95
 H       1.837880     1.108054     2.590101      20.97
 H       0.346613     2.414656     2.284533      20.55
 C       0.167422    -1.029623    -0.343510       7.39
 O      -1.177650    -1.412128    -0.051763     165.96
 C       0.837145    -1.426746    -1.558851      60.86
 H       0.136503    -2.112360    -2.182339      18.66
 C       2.674682     0.137605    -1.199934      37.89
 C       4.054304     0.528658    -1.624301      68.37
 H       4.105196     0.110276    -2.810689      20.75
 O       4.415041     1.918555    -1.604251     242.91
 H       4.799556     2.102639    -0.640004      20.94
 C       5.237351    -0.361632    -0.957018      78.18
 H       5.480558    -0.054919     0.116166      21.28
 O       4.730807    -1.766506    -0.843411     305.64
 H       4.831803    -2.146877    -1.838345      25.54
 C       6.651527    -0.218299    -1.593975      92.72
 O       7.215515     1.096166    -1.219000     280.15
 H       7.549716     0.948397    -0.253851      30.24
 H       6.611607    -0.362421    -2.676993      34.65
 H       7.197253    -1.248739    -1.308612      32.15
55
name= lig-ACN-Water-frame_210
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 C      -3.667743     0.058815    -3.121221      49.17
 H      -3.498837    -0.878748    -3.704795      20.68
 C      -3.735705     1.276332    -0.941750      54.37
 H      -3.644546     1.054731     0.100312      18.79
 C      -4.038005     2.521739    -1.591464      28.52
 O      -4.280157     3.738357    -1.039469     267.28
 C      -3.719937     4.192006     0.223037      99.79
 H      -2.622267     3.972169     0.215571      22.66
 H      -4.309157     3.590121     1.042015      24.31
 H      -4.167218     5.410796     0.329683      22.58
 C      -4.279939     2.487496    -2.986899      -0.74
 O      -4.797558     3.588046    -3.629757     322.27
 H      -4.265405     4.407514    -3.465462      23.90
 C      -4.029517     1.306340    -3.783831      32.56
 H      -4.067575     1.513670    -4.837918      21.21
 C      -3.622578     0.047556    -1.734576      18.35
 C      -3.401108    -1.304058    -1.034425      86.37
 H      -4.120907    -2.031594    -1.474688      23.25
 O      -4.026191    -1.289292     0.277572     182.83
 H      -3.324184    -0.853804     0.881257      21.82
 C      -2.039630    -2.052933    -0.983551      90.47
 H      -1.719244    -2.144300    -2.054174      22.06
 C      -2.223074    -3.551425    -0.612946     110.49
 O      -2.932266    -4.232547    -1.685565     237.65
 H      -2.267676    -4.657510    -2.364576      26.05
 H      -2.816444    -3.459809     0.276104      24.96
 H      -1.205028    -3.920202    -0.397793      24.09
 C       2.046595    -0.893871    -1.929242      10.66
 H       2.525020    -1.401305    -2.772734      17.80
 C       1.943163     0.629319    -0.049036      53.63
 H       2.254361     1.365699     0.528732      16.84
 C       0.772812     0.008369     0.413712      17.18
 O       0.076452     0.428849     1.563416     201.19
 C       0.650444     1.308827     2.604561      91.35
 H      -0.108688     0.929670     3.399954      21.05
 H       1.757525     1.122712     2.812510      23.19
 H       0.523209     2.481324     2.378070      21.36
 C       0.070771    -0.997406    -0.457077      14.84
 O      -1.170539    -1.401608    -0.009013     202.23
 C       0.762314    -1.472291    -1.554223      42.51
 H       0.567517    -2.403335    -2.198328      17.08
 C       2.626793     0.081639    -1.155207      53.35
 C       4.063656     0.495652    -1.655720      68.25
 H       4.120871     0.282885    -2.885759      21.31
 O       4.382171     1.900886    -1.568632     262.71
 H       4.798835     2.048646    -0.689570      24.06
 C       5.139428    -0.373592    -0.981655      98.49
 H       5.166190     0.039028     0.086979      19.50
 O       4.807919    -1.747185    -0.776573     295.60
 H       5.017755    -2.271079    -1.594981      29.54
 C       6.598368    -0.239376    -1.615106      94.20
 O       7.213337     1.035148    -1.140784     285.26
 H       7.760426     0.923542    -0.261815      29.45
 H       6.680130    -0.138943    -2.709167      32.30
 H       7.303648    -1.025195    -1.084132      27.85
55
name= lig-ACN-Water-frame_211
 C      -3.649708     0.130467    -3.131349      46.44
 H      -3.388284    -0.852353    -3.657502      22.13
 C      -3.732599     1.240257    -1.011833      59.93
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 H      -3.667169     1.351606     0.099977      15.85
 C      -4.022714     2.450277    -1.620435      39.18
 O      -4.257775     3.737344    -1.054172     258.09
 C      -3.760389     4.106251     0.222912     120.67
 H      -2.657161     4.050471     0.294548      24.71
 H      -4.154450     3.644708     1.176588      25.62
 H      -3.797303     5.407636     0.214625      22.91
 C      -4.233665     2.444437    -3.063310      19.67
 O      -4.749674     3.628192    -3.604276     274.68
 H      -4.329017     4.415134    -3.234094      23.95
 C      -4.103819     1.278129    -3.787393      82.10
 H      -4.273100     1.183698    -4.883395      25.97
 C      -3.512618     0.080812    -1.690709      23.80
 C      -3.458070    -1.288297    -1.046390      96.90
 H      -4.025468    -1.932170    -1.717971      23.70
 O      -3.943210    -1.321463     0.276565     194.86
 H      -3.366065    -1.029305     1.005595      19.51
 C      -2.117039    -1.995757    -1.067476      68.27
 H      -1.487346    -1.758058    -1.981017      21.11
 C      -2.190444    -3.465145    -0.600569     118.87
 O      -2.896876    -4.249504    -1.573083     247.44
 H      -2.327821    -4.397444    -2.347291      28.67
 H      -2.768872    -3.732508     0.296253      23.01
 H      -1.248234    -3.900969    -0.384512      24.61
 C       2.009497    -0.992121    -1.890869       7.38
 H       2.668828    -1.388042    -2.667621      17.45
 C       2.025375     0.642071    -0.001370      65.19
 H       2.584174     1.273130     0.549149      16.99
 C       0.758184     0.032074     0.362944       8.78
 O       0.071036     0.416256     1.521229     204.03
 C       0.601284     1.285131     2.618661      90.47
 H      -0.078468     1.314498     3.629700      21.04
 H       1.559647     0.904457     2.991803      22.98
 H       0.651020     2.363166     2.217031      21.53
 C       0.067920    -0.893844    -0.452063       6.07
 O      -1.174872    -1.396301     0.025386     165.17
 C       0.764625    -1.527972    -1.586198      40.63
 H       0.241693    -2.370144    -2.080339      15.84
 C       2.649902     0.096521    -1.193516      58.29
 C       4.017094     0.458796    -1.727867      67.49
 H       3.958774     0.316206    -2.928813      22.32
 O       4.348202     1.901322    -1.554335     239.02
 H       4.352097     2.031450    -0.604551      26.77
 C       5.150171    -0.363735    -0.962753     101.84
 H       5.169170     0.055542     0.091980      21.41
 O       4.879743    -1.778009    -0.752113     272.61
 H       4.768985    -2.055135    -1.652247      28.96
 C       6.555729    -0.167874    -1.505362      89.30
 O       7.246520     0.987716    -1.115142     298.79
 H       7.421908     0.861339    -0.125868      31.31
 H       6.390270    -0.215605    -2.614742      31.68
 H       7.122504    -1.187961    -1.395704      30.26
55
name= lig-ACN-Water-frame_212
 C      -3.626391     0.129281    -3.121520      62.87
 H      -3.533005    -0.749168    -3.844711      20.41
 C      -3.699811     1.310977    -0.921156      42.72
 H      -3.671483     1.259531     0.230809      18.00
 C      -4.009168     2.454257    -1.700966      26.36
 O      -4.259519     3.685544    -1.094468     234.85
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 C      -3.677983     4.059093     0.237091     100.39
 H      -2.674322     3.694879     0.373248      25.52
 H      -4.333337     3.599646     0.973497      25.79
 H      -3.976552     5.304518     0.325071      23.13
 C      -4.250306     2.509600    -3.086086      -2.60
 O      -4.691671     3.626522    -3.658360     245.37
 H      -4.276641     4.428779    -3.235389      26.14
 C      -4.118370     1.248280    -3.811673      47.02
 H      -4.435893     1.220911    -4.915675      22.93
 C      -3.441491     0.102113    -1.733045      14.03
 C      -3.448750    -1.304724    -1.061477      72.69
 H      -4.141167    -1.933167    -1.517686      25.30
 O      -3.954292    -1.343433     0.336431     137.98
 H      -3.271890    -0.815792     0.838032      24.01
 C      -2.015228    -1.939076    -1.022285      85.35
 H      -1.726882    -1.922147    -2.143472      23.29
 C      -2.146495    -3.435552    -0.593903     114.25
 O      -2.892150    -4.310662    -1.512081     266.32
 H      -2.564772    -4.143714    -2.392390      30.65
 H      -2.603361    -3.250484     0.403375      23.79
 H      -1.164347    -3.743281    -0.547162      25.83
 C       2.040442    -1.059113    -1.882120      82.02
 H       2.354163    -1.523143    -2.819265      13.29
 C       2.067361     0.519365    -0.020035      80.15
 H       2.438629     1.326163     0.631841      14.97
 C       0.764111     0.177926     0.369644      12.51
 O       0.009870     0.400089     1.540612     208.97
 C       0.605151     1.246882     2.543719      98.17
 H      -0.397358     1.360306     3.234489      20.94
 H       1.456926     0.778016     3.005560      24.22
 H       0.911228     2.226839     2.139242      23.74
 C       0.104081    -0.893619    -0.441846       2.02
 O      -1.204519    -1.344295    -0.002837     185.33
 C       0.733529    -1.489223    -1.489769      71.93
 H       0.274843    -2.182550    -2.130670      20.81
 C       2.605479     0.048815    -1.248233      38.89
 C       3.994140     0.483306    -1.706762      74.26
 H       4.217318     0.155737    -2.786906      23.45
 O       4.286633     1.883338    -1.556285     231.97
 H       4.528441     2.053166    -0.607616      24.96
 C       5.133916    -0.338356    -0.858283      62.63
 H       5.111053    -0.002815     0.205632      24.43
 O       4.897351    -1.794067    -0.807840     285.44
 H       4.732234    -2.249368    -1.695212      26.44
 C       6.515320    -0.179419    -1.541086      87.83
 O       7.304241     0.984752    -1.107233     262.71
 H       7.505757     1.016875    -0.149270      30.58
 H       6.483156     0.076335    -2.637465      29.44
 H       7.093983    -1.096191    -1.271650      29.74
55
name= lig-ACN-Water-frame_213
 C      -3.650292     0.110503    -3.129799      37.11
 H      -3.560937    -0.930087    -3.511172      20.29
 C      -3.622381     1.295859    -1.001457      58.84
 H      -3.621889     1.284851     0.140793      18.94
 C      -3.974427     2.489433    -1.629530      37.40
 O      -4.236574     3.720236    -1.091719     256.28
 C      -3.701305     3.939327     0.205066     123.02
 H      -2.664995     3.647220     0.274477      25.52
 H      -4.281530     3.548424     0.999863      27.08
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 H      -3.529720     5.180065     0.283507      23.42
 C      -4.245993     2.455391    -3.098453      28.00
 O      -4.656313     3.647288    -3.798663     185.33
 H      -4.291367     4.535300    -3.388354      20.64
 C      -4.100279     1.319420    -3.813171      62.41
 H      -4.235191     1.340584    -4.952505      25.08
 C      -3.494067     0.108808    -1.695881      17.17
 C      -3.384405    -1.278163    -0.983184     101.48
 H      -3.925277    -1.927216    -1.556048      26.43
 O      -3.972355    -1.314419     0.330244     176.38
 H      -3.589683    -0.789775     1.121602      19.83
 C      -2.028514    -1.982474    -1.046500      78.47
 H      -1.415477    -1.823858    -1.997081      22.32
 C      -2.033095    -3.434946    -0.609075     118.92
 O      -2.905485    -4.310659    -1.406124     212.30
 H      -2.552318    -4.467986    -2.372701      26.30
 H      -2.563620    -3.689998     0.347598      23.71
 H      -1.130273    -3.860816    -0.434071      26.56
 C       2.009830    -1.071512    -1.946378      62.23
 H       2.537213    -1.474812    -2.825416       9.18
 C       2.007586     0.482984    -0.035481      76.89
 H       2.718754     1.302554     0.413061      14.91
 C       0.676080     0.082074     0.360428      30.05
 O      -0.007542     0.408053     1.497316     235.66
 C       0.588522     1.257100     2.480593     109.83
 H      -0.244582     1.639256     3.284141      22.83
 H       1.289820     0.754080     3.105291      24.93
 H       1.021963     2.126869     2.070860      24.49
 C       0.073150    -0.881054    -0.349509      25.73
 O      -1.191834    -1.210015    -0.073865     162.97
 C       0.735614    -1.469174    -1.454490      75.38
 H       0.307916    -2.270764    -1.957044      21.91
 C       2.635830    -0.026467    -1.237962      49.07
 C       4.057989     0.418295    -1.584367      85.03
 H       4.143503     0.247748    -2.683289      22.24
 O       4.224685     1.890271    -1.555297     217.48
 H       4.739485     2.139572    -0.686798      25.27
 C       5.100072    -0.381446    -0.863083      97.42
 H       5.156198    -0.081068     0.184693      29.09
 O       4.850851    -1.784064    -0.868979     337.06
 H       4.994624    -1.963866    -1.903354      26.16
 C       6.566911    -0.117537    -1.534017      99.56
 O       7.345801     1.032238    -1.157419     279.27
 H       7.749070     0.860387    -0.286123      29.28
 H       6.321915    -0.182943    -2.641863      32.54
 H       7.138307    -1.026286    -1.405471      33.46
55
name= lig-ACN-Water-frame_214
 C      -3.742942     0.093526    -3.105324      90.41
 H      -3.624991    -0.709127    -3.800896      24.72
 C      -3.574074     1.322731    -1.025756      45.84
 H      -3.340511     1.381620     0.049378      18.60
 C      -3.999788     2.520447    -1.718002      27.90
 O      -4.217357     3.777053    -1.085287     268.98
 C      -3.632609     3.885305     0.228157     110.59
 H      -2.714169     3.310756     0.332076      25.40
 H      -4.255818     3.492576     0.985314      26.67
 H      -3.553337     5.097847     0.418644      23.86
 C      -4.216144     2.547917    -3.101543       4.51
 O      -4.594329     3.611133    -3.897915     262.53
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 H      -4.464645     4.506109    -3.340087      26.46
 C      -3.990789     1.254723    -3.787504      36.46
 H      -3.974872     1.265163    -4.903731      20.68
 C      -3.550817     0.063040    -1.709884      25.20
 C      -3.383875    -1.270341    -0.979309      84.82
 H      -3.998883    -1.865494    -1.522859      24.72
 O      -4.039203    -1.290336     0.314796     207.99
 H      -3.314654    -0.963291     0.978251      21.43
 C      -1.977715    -1.945367    -1.011745      81.48
 H      -1.796648    -1.872188    -2.131006      22.55
 C      -1.974337    -3.556864    -0.543627     108.94
 O      -2.898382    -4.299023    -1.359049     238.51
 H      -2.283173    -4.724247    -2.053595      27.03
 H      -2.238009    -3.370200     0.527424      23.75
 H      -1.022531    -3.873186    -0.718664      24.70
 C       1.985213    -1.012083    -1.955945      27.47
 H       2.456775    -1.633250    -2.733585      18.60
 C       1.952068     0.501940    -0.069548      79.20
 H       2.413390     1.291326     0.734257      16.33
 C       0.774700     0.022740     0.406013      10.93
 O      -0.058425     0.463834     1.491282     206.34
 C       0.614325     1.352129     2.473103     107.44
 H      -0.275734     1.818192     3.061732      23.40
 H       1.311441     0.761891     3.054399      24.91
 H       1.081517     2.100850     1.946721      24.96
 C       0.068322    -0.959064    -0.457706      -3.80
 O      -1.269074    -1.124774    -0.081517     162.91
 C       0.762260    -1.562864    -1.552190      62.43
 H       0.261574    -2.434814    -1.945425      18.06
 C       2.652126    -0.081496    -1.141389      49.44
 C       4.019293     0.399913    -1.578642      79.32
 H       4.143104     0.077697    -2.592383      22.23
 O       4.206970     1.874454    -1.526224     261.38
 H       4.383729     2.085630    -0.521473      23.37
 C       5.250838    -0.362115    -0.840379      88.45
 H       5.236671    -0.185265     0.226619      23.75
 O       4.807014    -1.776549    -0.972416     347.40
 H       4.794820    -2.247201    -1.904188      23.70
 C       6.596992    -0.131079    -1.516525     119.66
 O       7.364387     1.094393    -1.255999     286.68
 H       7.554599     1.131435    -0.250362      31.86
 H       6.498749     0.061408    -2.620133      32.57
 H       7.174463    -0.969646    -1.296265      31.23
55
name= lig-ACN-Water-frame_215
 C      -3.801868     0.042413    -3.101834      59.10
 H      -3.697146    -0.886864    -3.572069      28.23
 C      -3.586380     1.378844    -1.077174      54.86
 H      -3.324571     1.369101    -0.055063      19.97
 C      -4.003234     2.563274    -1.742264       9.06
 O      -4.170897     3.780935    -1.094414     214.65
 C      -3.571745     3.859278     0.292987     103.03
 H      -2.578051     3.393536     0.344577      25.27
 H      -4.363856     3.499611     0.964822      25.14
 H      -3.330971     4.986064     0.514084      24.31
 C      -4.154362     2.507201    -3.196366      17.91
 O      -4.520216     3.607968    -3.940741     198.79
 H      -4.274733     4.495286    -3.446343      23.70
 C      -3.908519     1.323913    -3.800637      60.31
 H      -3.994176     1.304638    -4.866333      18.79
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 C      -3.566376     0.072040    -1.715707      -2.69
 C      -3.522053    -1.374000    -1.038150      87.65
 H      -4.072583    -2.082241    -1.563955      24.16
 O      -4.079327    -1.259751     0.316706     197.03
 H      -3.474884    -0.948653     1.094592      20.63
 C      -2.091645    -1.973821    -0.970983      83.47
 H      -1.514399    -1.921745    -1.904107      21.76
 C      -1.916692    -3.456867    -0.518944     117.95
 O      -2.866335    -4.311786    -1.299959     269.34
 H      -2.413717    -4.761699    -1.983991      30.25
 H      -2.119159    -3.810511     0.525862      23.97
 H      -0.927653    -3.838629    -0.626443      23.92
 C       2.003647    -1.067315    -1.901229      38.03
 H       2.596542    -1.286325    -2.806728      16.31
 C       1.992049     0.524109     0.025330      68.63
 H       2.552191     1.427501     0.585966      15.23
 C       0.691297    -0.062176     0.398999       5.80
 O      -0.042014     0.519888     1.458394     201.79
 C       0.622776     1.460264     2.394846     109.10
 H      -0.204235     1.844008     3.017289      23.97
 H       1.311736     0.986508     3.144046      24.07
 H       1.115017     2.275225     1.997892      25.67
 C       0.079813    -0.978602    -0.460678      13.81
 O      -1.249790    -1.111464    -0.137010     174.90
 C       0.709688    -1.630128    -1.603091      76.37
 H       0.391001    -2.297028    -2.465900      17.27
 C       2.637486    -0.046845    -1.111459      29.27
 C       4.084936     0.419152    -1.572860      90.73
 H       4.165115     0.283908    -2.599501      20.85
 O       4.180956     1.833018    -1.455039     303.23
 H       4.232119     2.059239    -0.519283      25.02
 C       5.230799    -0.373810    -0.887279     102.30
 H       5.367899    -0.141567     0.151130      24.91
 O       4.826305    -1.779295    -0.999529     376.30
 H       4.895478    -1.933722    -1.963588      28.25
 C       6.696358    -0.132623    -1.574441     110.72
 O       7.350650     1.169672    -1.283285     236.51
 H       7.529015     1.152186    -0.246256      29.69
 H       6.506762    -0.323403    -2.652498      35.13
 H       7.326252    -0.885438    -1.258440      33.26
55
name= lig-ACN-Water-frame_216
 C      -3.782855     0.071349    -3.153768      62.32
 H      -3.930842    -0.839830    -3.654846      25.13
 C      -3.629485     1.313947    -1.088238      53.53
 H      -3.600944     1.442456    -0.052704      19.00
 C      -3.930671     2.546846    -1.739456      22.08
 O      -4.067595     3.786512    -1.066895     259.64
 C      -3.551383     3.877860     0.261305     111.05
 H      -2.558994     3.308791     0.376832      22.41
 H      -4.128335     3.428832     1.156710      23.64
 H      -3.461994     4.979422     0.380649      24.14
 C      -4.072245     2.530827    -3.176465      -0.54
 O      -4.415329     3.655845    -3.958523     282.90
 H      -4.081333     4.537868    -3.603633      25.38
 C      -3.900173     1.231064    -3.914017      59.50
 H      -3.997454     1.262670    -4.950476      19.82
 C      -3.630748     0.066836    -1.729664      25.11
 C      -3.589701    -1.354638    -0.982405      79.20
 H      -4.259346    -2.001351    -1.533150      23.55
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 O      -4.160714    -1.263240     0.322071     216.39
 H      -3.494254    -0.677453     0.772574      24.26
 C      -2.137988    -2.006064    -0.974928      85.98
 H      -2.014659    -1.993626    -2.061040      24.16
 C      -1.941266    -3.453725    -0.500622     114.54
 O      -2.814429    -4.324258    -1.236802     262.44
 H      -2.386013    -4.434336    -2.141093      29.30
 H      -2.227922    -3.422867     0.574754      24.67
 H      -0.861421    -3.574710    -0.701001      24.70
 C       2.074634    -1.076066    -1.832020      34.07
 H       2.425007    -1.441966    -2.802447      14.64
 C       2.002120     0.410528     0.066283      59.03
 H       2.419148     1.289387     0.636604      12.61
 C       0.759199     0.034625     0.372367      23.72
 O      -0.005942     0.557322     1.414234     226.34
 C       0.587310     1.555038     2.331435     101.36
 H      -0.188906     1.909660     2.888370      24.79
 H       1.388807     0.972181     2.876436      22.46
 H       0.942418     2.333373     1.691142      23.51
 C       0.062463    -1.035007    -0.476337       8.10
 O      -1.288612    -1.143501    -0.158703     172.85
 C       0.754928    -1.513442    -1.593128      67.77
 H      -0.001453    -2.100563    -2.243694      16.05
 C       2.663484    -0.041003    -1.125974      52.33
 C       4.048227     0.439461    -1.575820      93.43
 H       4.091959     0.258377    -2.573793      26.53
 O       4.178252     1.887571    -1.338300     263.23
 H       4.632895     1.990001    -0.504459      27.54
 C       5.249220    -0.384397    -0.974551      76.09
 H       5.233822    -0.138270     0.078196      26.27
 O       4.919009    -1.760777    -0.979838     392.35
 H       4.894426    -2.208536    -1.792861      33.83
 C       6.729036    -0.149116    -1.589732     107.27
 O       7.281744     1.194451    -1.296482     258.25
 H       7.690752     1.094913    -0.393858      31.43
 H       6.819518    -0.183295    -2.678360      34.28
 H       7.330156    -0.889891    -1.169561      34.29
55
name= lig-ACN-Water-frame_217
 C      -3.772060     0.046702    -3.207006      51.54
 H      -3.774801    -0.845925    -3.828142      22.23
 C      -3.718582     1.276147    -1.027095      36.27
 H      -3.695887     1.112070     0.031339      18.54
 C      -3.822935     2.501677    -1.769518      43.11
 O      -3.978607     3.734261    -1.107178     213.63
 C      -3.479467     3.919538     0.247404     122.23
 H      -2.433038     3.465749     0.365070      23.11
 H      -4.380302     3.476826     0.905533      24.43
 H      -3.375240     4.962123     0.471600      24.39
 C      -3.965228     2.535719    -3.254394      23.96
 O      -4.266452     3.661743    -3.946104     200.41
 H      -4.139925     4.439724    -3.352738      24.43
 C      -3.964135     1.316050    -3.905185      63.83
 H      -4.032397     1.249156    -4.953849      23.87
 C      -3.698818     0.006871    -1.778570       1.59
 C      -3.632429    -1.267213    -0.960264      89.61
 H      -4.264700    -2.039204    -1.489314      22.79
 O      -4.225746    -1.234442     0.372748     176.28
 H      -3.762875    -0.759901     1.101849      22.91
 C      -2.223755    -1.952687    -1.072629      77.36
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 H      -1.810071    -1.889184    -2.063004      23.20
 C      -2.014510    -3.392279    -0.463073     110.27
 O      -2.762431    -4.382009    -1.202782     254.70
 H      -2.448669    -4.315290    -2.194530      26.75
 H      -2.274231    -3.487533     0.598507      24.04
 H      -0.950078    -3.840285    -0.425309      22.40
 C       2.066381    -1.094456    -1.895878      29.00
 H       2.661642    -1.583501    -2.664346      12.59
 C       2.108528     0.385894     0.037509      56.87
 H       2.588641     1.052784     0.670950      13.21
 C       0.696068     0.019071     0.347026      23.13
 O      -0.022995     0.570285     1.379699     235.09
 C       0.564222     1.616916     2.192169     124.60
 H      -0.128220     1.849370     2.838210      25.98
 H       1.450803     1.356704     2.850330      23.47
 H       0.886296     2.555893     1.686890      23.64
 C       0.050582    -0.896004    -0.403124      25.49
 O      -1.329346    -1.186129    -0.196127     195.52
 C       0.732918    -1.389702    -1.523200      84.93
 H       0.423097    -2.193922    -2.280686      20.00
 C       2.746947    -0.113187    -1.090597      48.67
 C       4.033124     0.506668    -1.623772      86.32
 H       3.997559     0.549131    -2.613907      22.59
 O       4.211876     1.936182    -1.245182     222.47
 H       4.520122     2.044638    -0.264289      20.71
 C       5.289674    -0.349652    -1.040464     105.88
 H       5.451850    -0.012842    -0.021376      22.97
 O       5.024761    -1.817316    -0.933846     350.45
 H       4.947625    -2.105829    -1.805422      33.85
 C       6.693220    -0.122862    -1.575499     106.33
 O       7.215157     1.191653    -1.288075     312.38
 H       7.501719     1.244534    -0.381555      33.19
 H       6.657968    -0.289631    -2.642714      32.72
 H       7.310818    -0.872738    -1.123005      32.39
55
name= lig-ACN-Water-frame_218
 C      -3.799904     0.078380    -3.224984      72.93
 H      -3.555269    -0.900542    -3.731854      25.10
 C      -3.806220     1.210343    -1.111855      60.39
 H      -3.743327     1.393817    -0.019258      15.58
 C      -3.746661     2.444442    -1.764032      51.42
 O      -3.857199     3.706620    -1.213639     207.05
 C      -3.449671     3.930831     0.211307     120.20
 H      -2.417952     3.404051     0.504070      23.54
 H      -4.124304     3.423548     1.078019      26.41
 H      -3.409089     4.936908     0.245736      27.73
 C      -3.889394     2.498079    -3.162154       7.66
 O      -4.111535     3.666065    -3.926449     158.22
 H      -4.023475     4.554748    -3.504201      21.96
 C      -3.968397     1.281427    -3.887473      64.48
 H      -4.143492     1.430036    -4.955487      22.99
 C      -3.766878     0.055991    -1.793379      20.00
 C      -3.664013    -1.299163    -1.001507      43.73
 H      -4.377143    -2.089828    -1.466731      21.79
 O      -4.274838    -1.194714     0.426803     130.09
 H      -3.442826    -0.994992     0.951609      24.17
 C      -2.175487    -1.918439    -1.051092      84.90
 H      -1.915796    -1.902120    -2.074089      25.25
 C      -2.119717    -3.367499    -0.462749     100.04
 O      -2.771832    -4.461307    -1.193423     235.03
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 H      -2.333540    -4.669026    -2.043307      28.32
 H      -2.686392    -3.314651     0.460963      24.18
 H      -0.957306    -3.346799    -0.312559      22.04
 C       2.077338    -1.044874    -1.880194      24.65
 H       2.400541    -1.578471    -2.765316      21.49
 C       2.085444     0.379564     0.063770      85.54
 H       2.589188     1.004352     0.643112      18.73
 C       0.767662     0.072023     0.377119       5.36
 O      -0.032252     0.612976     1.390092     206.68
 C       0.538634     1.723440     2.131226     109.75
 H      -0.116045     1.977572     2.805221      26.49
 H       1.475876     1.297109     2.534959      23.26
 H       0.623815     2.548807     1.337848      23.57
 C      -0.032153    -0.840100    -0.545502      -3.35
 O      -1.322725    -1.125004    -0.159311     168.38
 C       0.739055    -1.438554    -1.568684      55.07
 H       0.138112    -2.225402    -2.053508      18.05
 C       2.783686    -0.156205    -1.115420      50.74
 C       4.145735     0.560806    -1.598752      82.03
 H       4.155080     0.585721    -2.564636      24.59
 O       4.231468     1.948967    -1.184532     248.50
 H       4.100940     1.991568    -0.151599      21.95
 C       5.272883    -0.338118    -0.996535     105.83
 H       5.173032    -0.079938     0.057359      22.57
 O       5.104334    -1.791098    -0.919872     304.04
 H       5.117896    -2.305791    -1.770342      27.49
 C       6.670140    -0.115561    -1.622177     104.71
 O       7.167898     1.227456    -1.282093     273.23
 H       7.369454     1.114422    -0.315626      30.47
 H       6.734111    -0.194735    -2.677306      31.97
 H       7.379702    -0.891003    -1.224601      31.53
55
name= lig-ACN-Water-frame_219
 C      -3.824861     0.027993    -3.194987      44.17
 H      -3.851193    -0.881167    -3.923038      20.57
 C      -3.826743     1.282272    -1.071150      41.37
 H      -3.953286     1.071951     0.032816      20.95
 C      -3.759825     2.472840    -1.790334      34.91
 O      -3.700336     3.723531    -1.208035     224.90
 C      -3.405933     3.907346     0.119600     122.02
 H      -2.323448     3.447037     0.318696      25.52
 H      -4.297259     3.532591     0.816852      26.12
 H      -3.373864     4.919112     0.295972      27.16
 C      -3.884001     2.492081    -3.191974      16.18
 O      -3.949631     3.608766    -3.912629      45.01
 H      -3.853745     4.361013    -3.296732      20.24
 C      -3.928959     1.281654    -3.897114      63.05
 H      -3.982637     1.225612    -5.031369      23.59
 C      -3.822790    -0.048372    -1.795267     -44.90
 C      -3.702952    -1.331650    -1.001230      66.22
 H      -4.290567    -2.179690    -1.608251      22.76
 O      -4.214752    -1.164555     0.361711     168.04
 H      -3.582486    -0.854789     1.107919      21.64
 C      -2.255204    -1.887849    -1.013224      87.04
 H      -1.860941    -1.824352    -1.981086      26.39
 C      -2.226145    -3.347727    -0.446955     114.31
 O      -2.771554    -4.494607    -1.186917     238.91
 H      -2.052019    -4.790039    -1.725464      28.00
 H      -2.753066    -3.334366     0.515020      24.22
 H      -1.250655    -3.898788    -0.085193      21.14
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 C       2.024201    -1.078709    -1.919468      96.22
 H       2.562701    -1.288998    -2.840078      14.51
 C       2.088747     0.386086     0.060279      43.45
 H       2.475653     1.085560     0.727816      11.35
 C       0.697323     0.073799     0.300071      16.55
 O      -0.031931     0.618612     1.380911     206.71
 C       0.530619     1.824340     2.058275     111.03
 H      -0.097532     2.085353     2.829393      25.67
 H       1.506329     1.745919     2.520836      24.48
 H       0.679667     2.736645     1.350698      24.20
 C       0.053872    -0.757558    -0.581064      13.94
 O      -1.332535    -1.032911    -0.150155     144.51
 C       0.685872    -1.502148    -1.614010      74.39
 H       0.288965    -2.135698    -2.335641      21.86
 C       2.747390    -0.042755    -1.131913      41.63
 C       4.133220     0.478653    -1.535591      90.08
 H       4.263749     0.461205    -2.493962      22.94
 O       4.208966     1.933493    -1.159138     179.29
 H       4.547609     1.970028    -0.156290      22.68
 C       5.334562    -0.363166    -0.916719      96.29
 H       5.583958    -0.063123     0.107698      27.46
 O       5.103677    -1.758610    -0.922854     315.61
 H       5.095798    -2.055617    -1.966505      28.93
 C       6.677968    -0.049737    -1.633695     105.11
 O       7.152276     1.257208    -1.268546     227.10
 H       7.579874     1.220209    -0.317879      30.13
 H       6.508258    -0.040306    -2.692374      36.57
 H       7.410797    -0.871684    -1.300512      34.46
55
name= lig-ACN-Water-frame_220
 C      -3.898028    -0.019818    -3.200927      71.99
 H      -4.047026    -1.062763    -3.683240      24.47
 C      -3.832172     1.188349    -1.066738      59.65
 H      -3.851317     1.367798     0.035057      19.44
 C      -3.810969     2.443184    -1.764820      24.58
 O      -3.577538     3.790062    -1.313536     164.30
 C      -3.332943     3.897475     0.147558     116.57
 H      -2.450618     3.267286     0.629559      23.82
 H      -4.205310     3.361119     0.720040      24.80
 H      -3.209180     4.937150     0.381339      26.62
 C      -3.873555     2.410320    -3.235130       1.11
 O      -3.792036     3.628102    -3.941062      45.11
 H      -3.874876     4.514991    -3.455999      21.20
 C      -3.865515     1.179487    -3.895776      60.78
 H      -3.832832     1.279912    -5.044000      20.11
 C      -3.862463     0.012098    -1.772884      26.59
 C      -3.677337    -1.309143    -0.986363      66.07
 H      -4.387349    -2.208040    -1.348476      23.87
 O      -4.197763    -1.174375     0.306721     155.13
 H      -3.506604    -0.641976     0.771586      25.48
 C      -2.233200    -1.899549    -0.987562      79.03
 H      -1.943167    -1.965494    -2.018054      27.06
 C      -2.275475    -3.418791    -0.294053      93.27
 O      -2.803144    -4.465371    -1.195589     190.52
 H      -2.108352    -4.880651    -1.845650      25.81
 H      -2.997646    -3.399458     0.542228      24.74
 H      -1.131502    -3.361093    -0.018256      23.50
 C       2.048069    -0.981675    -1.954354      26.90
 H       2.480985    -1.531665    -2.790288      17.48
 C       2.023883     0.450931     0.033521      53.38
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 H       2.732844     1.101276     0.645531      13.68
 C       0.702113     0.151111     0.264002      15.82
 O       0.022632     0.649695     1.357029     209.44
 C       0.533432     1.914575     1.987983     101.81
 H      -0.309577     2.088192     2.687246      23.95
 H       1.429594     1.655965     2.461014      24.40
 H       0.464236     2.733323     1.184426      24.37
 C      -0.053838    -0.872463    -0.569722      -3.14
 O      -1.359779    -0.972068    -0.212592     152.10
 C       0.716571    -1.422849    -1.684824      58.96
 H       0.197844    -2.059201    -2.275053      22.16
 C       2.622175    -0.058322    -1.147926      38.64
 C       4.090703     0.436978    -1.424865      89.82
 H       4.125087     0.330907    -2.397889      26.56
 O       4.200851     1.868942    -1.156129     224.72
 H       4.595270     1.975408    -0.279025      26.94
 C       5.415038    -0.339864    -0.837809      75.55
 H       5.446377    -0.156733     0.262178      24.36
 O       5.064509    -1.756738    -0.937672     341.91
 H       4.920392    -2.214502    -1.945631      23.40
 C       6.655381     0.020071    -1.642680     104.95
 O       7.200013     1.322212    -1.266707     219.82
 H       7.458525     1.177406    -0.247845      28.09
 H       6.464856     0.038454    -2.714434      34.07
 H       7.499580    -0.812034    -1.568656      32.27
55
name= lig-ACN-Water-frame_221
 C      -3.982448    -0.062974    -3.154518      58.64
 H      -3.883611    -1.052497    -3.690613      27.21
 C      -3.823306     1.290172    -1.069429      45.29
 H      -3.572855     1.141830    -0.040165      20.04
 C      -3.815022     2.466120    -1.830773      18.17
 O      -3.469503     3.741037    -1.344266     216.63
 C      -3.306874     3.835367     0.177848      94.86
 H      -2.305468     3.249129     0.356087      24.37
 H      -4.224809     3.608130     0.749099      26.32
 H      -3.161287     4.952720     0.349858      25.23
 C      -3.818712     2.426392    -3.221903       1.58
 O      -3.656873     3.583332    -4.005996     144.84
 H      -3.640755     4.389136    -3.350975      23.39
 C      -3.839130     1.144189    -3.939333      36.47
 H      -3.824474     1.075099    -5.075247      18.28
 C      -3.874605    -0.016146    -1.766611      -5.63
 C      -3.685274    -1.308434    -1.027477      74.07
 H      -4.317479    -2.058932    -1.734288      21.12
 O      -4.200134    -1.167470     0.377314     166.06
 H      -3.579801    -0.724571     1.007809      22.43
 C      -2.259027    -1.998942    -0.958153      93.77
 H      -1.851887    -2.222870    -1.952053      24.12
 C      -2.271225    -3.370213    -0.242231     106.36
 O      -2.813649    -4.390186    -1.160158     190.98
 H      -2.137170    -4.434564    -1.925548      26.43
 H      -2.938532    -3.324499     0.671348      23.46
 H      -1.310491    -3.907908     0.201609      22.21
 C       1.970404    -0.966893    -2.012712      71.53
 H       2.617790    -1.402667    -2.784778      18.22
 C       1.958609     0.503960    -0.075367      74.78
 H       2.359632     1.258279     0.783303      15.41
 C       0.642778     0.129260     0.240558      19.39
 O       0.026091     0.695845     1.344223     243.97
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 C       0.463880     1.913256     1.905603     113.09
 H      -0.244144     2.367732     2.732098      23.32
 H       1.396978     1.924357     2.402486      24.38
 H       0.685993     2.713754     1.144322      24.52
 C       0.015839    -0.829572    -0.534288      18.58
 O      -1.431123    -0.998767    -0.318150     173.47
 C       0.628597    -1.312554    -1.697039      73.56
 H       0.237313    -2.071454    -2.283119      21.32
 C       2.722325    -0.062095    -1.089977      47.01
 C       4.095099     0.413602    -1.392832      98.28
 H       4.282268     0.347485    -2.367997      23.16
 O       4.203326     1.832761    -1.162677     284.20
 H       4.209461     1.976881    -0.230597      26.00
 C       5.259325    -0.379364    -0.841862     101.03
 H       5.539246    -0.172394     0.231829      23.54
 O       5.042268    -1.781192    -0.909609     340.08
 H       5.042652    -2.067118    -1.931780      26.32
 C       6.642989     0.087324    -1.653137      81.79
 O       7.240114     1.367250    -1.276504     260.35
 H       7.565891     1.299044    -0.294094      27.75
 H       6.325877     0.261532    -2.712624      34.01
 H       7.417100    -0.816824    -1.463505      30.97
55
name= lig-ACN-Water-frame_222
 C      -3.973648    -0.015436    -3.165310      71.91
 H      -3.980923    -0.945511    -3.703213      25.32
 C      -3.770436     1.272920    -1.123732      53.09
 H      -3.625082     1.426819    -0.108240      19.61
 C      -3.723509     2.479563    -1.860627      28.75
 O      -3.417606     3.680548    -1.264665     207.52
 C      -3.258743     3.810372     0.074625     114.77
 H      -2.500017     3.134718     0.623866      23.85
 H      -4.140406     3.476150     0.589774      26.90
 H      -2.941544     4.959635     0.276584      23.08
 C      -3.755448     2.387475    -3.356590      21.14
 O      -3.537209     3.524211    -4.050159     111.80
 H      -3.394981     4.309907    -3.441130      25.49
 C      -3.895304     1.155404    -3.899557      70.83
 H      -3.834521     1.128034    -4.987926      21.05
 C      -3.849048     0.028599    -1.747292      13.22
 C      -3.714041    -1.346079    -0.950712      59.74
 H      -4.527203    -2.199060    -1.240303      20.53
 O      -4.233610    -1.208158     0.407636     163.69
 H      -3.421587    -0.879470     0.927219      22.80
 C      -2.238383    -2.039037    -0.975909      82.05
 H      -1.989131    -2.205579    -2.064044      24.52
 C      -2.287297    -3.384358    -0.178297     110.52
 O      -2.837619    -4.289807    -1.124447     203.15
 H      -2.401252    -4.321777    -1.956770      29.42
 H      -3.037377    -3.335379     0.688235      23.70
 H      -1.161346    -3.557890     0.141759      23.38
 C       1.982618    -0.921645    -1.948923      62.13
 H       2.276616    -1.296281    -2.929859      22.01
 C       1.924723     0.546035    -0.105440      99.69
 H       2.498874     1.447715     0.458011      14.68
 C       0.619234     0.145797     0.269242      14.76
 O      -0.078614     0.694310     1.348752     214.98
 C       0.497540     2.007955     1.849963      87.50
 H      -0.521333     2.283489     2.475890      21.39
 H       1.334020     1.736220     2.442697      22.47
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 H       0.507390     2.693097     1.004975      23.33
 C      -0.116843    -0.788976    -0.597098      16.19
 O      -1.407794    -1.011505    -0.364300     181.51
 C       0.619271    -1.277011    -1.725501      33.72
 H       0.031680    -1.854296    -2.462167      17.42
 C       2.664693    -0.104658    -1.120463      50.41
 C       4.101397     0.426191    -1.495100      69.20
 H       4.087854     0.359998    -2.508873      23.74
 O       4.210281     1.859591    -1.141674     252.29
 H       4.215691     1.942523    -0.121936      23.85
 C       5.283918    -0.362635    -0.847900      89.83
 H       5.265058    -0.075671     0.258914      23.65
 O       5.033430    -1.813950    -0.875061     308.22
 H       4.964215    -2.210015    -1.809017      27.13
 C       6.542254     0.128027    -1.602188     100.60
 O       7.243633     1.365192    -1.293050     279.12
 H       7.668918     1.216884    -0.401660      29.65
 H       6.377329     0.103758    -2.749375      33.09
 H       7.343265    -0.786347    -1.520270      30.79
55
name= lig-ACN-Water-frame_223
 C      -3.932347    -0.036910    -3.145612      32.49
 H      -4.183157    -0.942916    -3.591332      21.24
 C      -3.696963     1.245142    -1.132359      58.58
 H      -3.808811     1.288001    -0.097857      22.10
 C      -3.585992     2.395388    -1.903265      20.10
 O      -3.370812     3.662378    -1.366458     220.56
 C      -3.234139     3.756145     0.165067      97.22
 H      -2.363405     3.116152     0.502828      22.83
 H      -4.138775     3.706493     0.653814      25.31
 H      -3.013221     4.978112     0.304831      22.67
 C      -3.688552     2.425570    -3.279499      19.11
 O      -3.422707     3.532289    -4.137032     154.55
 H      -3.469923     4.341345    -3.619909      24.57
 C      -3.958628     1.166470    -3.977374      53.16
 H      -4.037204     1.104086    -5.028172      27.23
 C      -3.823876    -0.050846    -1.725547       3.75
 C      -3.780960    -1.364626    -0.882789      86.36
 H      -4.417835    -2.118322    -1.590877      22.94
 O      -4.216026    -1.245926     0.461337     181.25
 H      -3.713366    -0.535517     1.037081      19.80
 C      -2.339247    -1.941135    -0.960181      90.56
 H      -2.009607    -2.176798    -2.040582      25.76
 C      -2.239048    -3.298253    -0.210146     108.54
 O      -2.903822    -4.289505    -1.096034     153.53
 H      -2.236789    -4.424726    -1.822328      27.95
 H      -2.858258    -3.274047     0.755284      24.51
 H      -1.176238    -3.632252     0.149725      23.88
 C       1.914782    -0.990135    -2.003585      47.76
 H       2.500618    -1.282957    -2.869038      18.69
 C       1.905352     0.546412    -0.059709      77.59
 H       2.388710     1.428303     0.483574      12.01
 C       0.571801     0.162803     0.240841      14.18
 O      -0.152822     0.719373     1.312817     229.48
 C       0.392424     2.002880     1.804991     105.77
 H      -0.310180     2.662287     2.609692      21.51
 H       1.349914     1.915555     2.350581      23.85
 H       0.744017     2.631562     1.041092      25.69
 C      -0.101124    -0.708085    -0.663404      21.02
 O      -1.450421    -1.007632    -0.327904     182.27
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 C       0.583893    -1.264259    -1.763008      66.03
 H       0.025921    -1.761008    -2.662476      20.75
 C       2.618895    -0.008112    -1.158399      75.23
 C       3.987770     0.472805    -1.550749      80.83
 H       4.198833     0.493004    -2.588346      22.27
 O       4.214669     1.885663    -1.139255     124.23
 H       4.579761     1.867211    -0.155085      24.74
 C       5.225005    -0.304856    -0.877123      91.49
 H       5.307804    -0.052623     0.241838      26.40
 O       5.054964    -1.787059    -0.825129     277.57
 H       4.947056    -2.155048    -1.705234      31.63
 C       6.574581     0.038441    -1.605075      89.12
 O       7.204784     1.328678    -1.294141     207.83
 H       7.538133     1.201209    -0.380214      30.70
 H       6.244602     0.174859    -2.728151      31.67
 H       7.369241    -0.840523    -1.365633      32.00
55
name= lig-ACN-Water-frame_224
 C      -3.962440    -0.074759    -3.171082      84.40
 H      -4.107339    -0.938778    -3.722144      22.35
 C      -3.649314     1.171048    -1.079972      63.89
 H      -3.604758     1.212637     0.006715      22.05
 C      -3.466371     2.392508    -1.865843      -5.74
 O      -3.317132     3.679065    -1.359332     150.87
 C      -3.229022     3.756155     0.137767     100.84
 H      -2.497260     3.047201     0.483842      26.39
 H      -4.073936     3.442766     0.616737      28.05
 H      -2.771675     4.936399     0.330523      23.54
 C      -3.615383     2.382256    -3.414740       5.12
 O      -3.361025     3.524301    -4.149820      71.11
 H      -3.635435     4.320200    -3.623043      24.61
 C      -3.958529     1.142365    -3.914439      69.22
 H      -4.208323     1.105283    -4.927557      22.85
 C      -3.816247    -0.057303    -1.768252      24.31
 C      -3.786181    -1.310380    -0.925304      73.09
 H      -4.554805    -2.169724    -1.234561      22.50
 O      -4.269146    -1.269263     0.502165     130.76
 H      -3.494357    -0.813470     1.078392      22.09
 C      -2.348813    -1.885555    -0.940005      88.18
 H      -2.114670    -1.893533    -2.079559      26.21
 C      -2.229249    -3.242447    -0.269355     115.58
 O      -2.928327    -4.300838    -1.055816     163.45
 H      -2.274301    -4.752539    -1.721530      27.63
 H      -2.689099    -3.187624     0.769298      25.74
 H      -1.166720    -3.562825    -0.266265      25.74
 C       1.941531    -0.933364    -2.034644      54.47
 H       2.427507    -1.496402    -2.811950      19.66
 C       1.882106     0.532432    -0.047013      52.39
 H       2.362087     1.142443     0.647041      15.32
 C       0.530473     0.220324     0.190662      11.01
 O      -0.204231     0.787827     1.260210     212.01
 C       0.370051     2.005041     1.774965      98.69
 H      -0.629438     2.409683     2.396886      22.23
 H       1.198984     1.698934     2.481373      23.04
 H       0.474313     2.657980     0.975881      26.54
 C      -0.168781    -0.701986    -0.679540       7.10
 O      -1.462709    -0.923278    -0.252267     164.06
 C       0.528456    -1.260166    -1.857688      71.41
 H      -0.070848    -2.134424    -2.437579      19.33
 C       2.512803     0.045437    -1.218431      24.32
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 C       3.989452     0.548897    -1.505066      96.73
 H       3.969553     0.464991    -2.610110      24.73
 O       4.214242     1.918563    -1.167008     211.19
 H       4.425554     2.036165    -0.209280      26.55
 C       5.140679    -0.314422    -0.914198      87.07
 H       5.276142     0.140275     0.114692      27.41
 O       5.063267    -1.694354    -0.764289     286.41
 H       5.023649    -2.000359    -1.680464      29.32
 C       6.574612    -0.021271    -1.636457      84.27
 O       7.158203     1.268339    -1.266644     185.28
 H       7.630891     1.213839    -0.384222      27.96
 H       6.604400    -0.134656    -2.834696      30.82
 H       7.281080    -0.930488    -1.313019      32.75
55
name= lig-ACN-Water-frame_225
 C      -4.028163    -0.095741    -3.185922      18.27
 H      -4.131406    -1.064378    -3.649407      25.83
 C      -3.578243     1.240163    -1.159412      59.99
 H      -3.372878     1.250820    -0.041863      21.67
 C      -3.437978     2.380761    -1.910002      20.40
 O      -3.253696     3.673276    -1.309350     214.15
 C      -3.187990     3.708511     0.065193     120.19
 H      -2.425956     3.132353     0.492411      26.65
 H      -4.125873     3.546347     0.467526      27.39
 H      -3.083215     4.938760     0.480299      23.24
 C      -3.526349     2.329024    -3.271660      24.25
 O      -3.361708     3.489638    -4.126230     110.91
 H      -3.524803     4.353098    -3.573727      20.53
 C      -3.923031     1.102400    -3.940934      30.00
 H      -4.025641     1.041675    -5.016770      30.87
 C      -3.859447    -0.009512    -1.748667     -18.76
 C      -3.800877    -1.342656    -0.872447      97.79
 H      -4.404905    -2.116154    -1.521390      23.77
 O      -4.302419    -1.220357     0.470819     147.21
 H      -3.615987    -1.105935     1.207743      22.51
 C      -2.342565    -1.821509    -0.980204      87.95
 H      -1.913775    -1.931230    -2.055531      28.05
 C      -2.160787    -3.269565    -0.359338     117.63
 O      -2.940053    -4.275462    -1.016104     224.23
 H      -2.362399    -4.708735    -1.631970      30.85
 H      -2.514049    -3.317859     0.700153      26.16
 H      -1.096229    -3.434024    -0.286511      27.04
 C       1.818410    -0.860400    -2.063258      24.73
 H       2.409016    -1.293109    -2.850759      21.41
 C       1.832542     0.529099    -0.079849      66.34
 H       2.393442     1.026896     0.564251      19.29
 C       0.479482     0.248087     0.121067      21.80
 O      -0.244294     0.798241     1.145624     215.68
 C       0.261809     2.020316     1.795013     107.55
 H      -0.580507     2.449783     2.510272      23.03
 H       1.213461     1.901250     2.453505      24.23
 H       0.651239     2.747035     1.137856      26.56
 C      -0.195195    -0.684808    -0.710625      13.33
 O      -1.502073    -0.874769    -0.221436     165.64
 C       0.498751    -1.254715    -1.779014      75.98
 H       0.166337    -2.193708    -2.431706      21.26
 C       2.530305     0.062710    -1.228033      63.58
 C       3.945635     0.547726    -1.534992      82.67
 H       4.146418     0.626347    -2.666062      20.72
 O       4.195737     2.004820    -1.198317     212.93
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 H       4.153018     2.083061    -0.261854      26.12
 C       5.222772    -0.199439    -0.928824      85.87
 H       5.332837     0.129544     0.133607      21.46
 O       4.993417    -1.670732    -0.733233     285.30
 H       4.853698    -2.276020    -1.544051      28.55
 C       6.537856    -0.052182    -1.595583      92.43
 O       7.157477     1.216088    -1.274158     241.61
 H       7.454641     1.054480    -0.297342      28.46
 H       6.488853    -0.143222    -2.772212      29.28
 H       7.195890    -0.857166    -1.084019      29.88
55
name= lig-ACN-Water-frame_226
 C      -4.071724    -0.067002    -3.112447      20.69
 H      -4.421718    -1.007869    -3.625387      18.98
 C      -3.507957     1.236566    -1.169036      53.42
 H      -3.370840     1.271072    -0.019842      20.34
 C      -3.436176     2.438770    -1.890688      18.28
 O      -3.158606     3.653286    -1.392369     187.12
 C      -3.208214     3.707915     0.162772      84.01
 H      -2.366687     3.207989     0.561329      25.13
 H      -4.075419     3.269272     0.560709      26.08
 H      -2.984772     4.943627     0.199225      21.66
 C      -3.533434     2.323683    -3.326026      13.89
 O      -3.394749     3.416292    -4.051228     106.85
 H      -3.297698     4.211934    -3.468000      23.75
 C      -3.813772     1.086586    -3.936351      47.69
 H      -3.779296     1.161042    -5.059242      22.53
 C      -3.923673    -0.029890    -1.732608      33.81
 C      -3.787873    -1.288247    -0.944092      93.59
 H      -4.440645    -2.116450    -1.359922      23.29
 O      -4.356071    -1.185398     0.400294     200.86
 H      -3.725128    -0.620161     0.914412      25.40
 C      -2.312701    -1.858902    -0.968320      88.09
 H      -2.162049    -1.753852    -2.103560      24.22
 C      -2.046874    -3.243166    -0.355452     120.67
 O      -2.939502    -4.256347    -1.024618     220.41
 H      -2.477187    -4.536452    -1.841418      30.51
 H      -2.331134    -3.141713     0.701813      25.47
 H      -1.091221    -3.662809    -0.467711      25.29
 C       1.780858    -0.766569    -2.094646      66.88
 H       2.129345    -1.102081    -3.066981      24.30
 C       1.859321     0.571270    -0.123686      69.13
 H       2.182385     1.273759     0.557904      15.50
 C       0.486404     0.300089     0.075009       8.93
 O      -0.305142     0.862936     1.093714     211.74
 C       0.205933     2.033785     1.826262     103.27
 H      -0.637232     2.434026     2.405259      24.36
 H       1.013978     1.586487     2.541498      22.14
 H       0.415104     2.775852     1.059814      23.90
 C      -0.250351    -0.653570    -0.670360      13.24
 O      -1.542860    -0.897147    -0.271439     195.01
 C       0.492998    -1.302861    -1.714013      64.92
 H      -0.126130    -1.925608    -2.457963      16.68
 C       2.553256     0.058199    -1.238627      43.53
 C       4.005472     0.619884    -1.591713      56.24
 H       4.076761     0.466026    -2.786336      19.63
 O       4.110397     2.069125    -1.230343     195.23
 H       4.326929     2.114051    -0.236802      23.03
 C       5.145203    -0.219425    -0.846853     100.04
 H       5.245312     0.240583     0.153706      23.94
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 O       4.878253    -1.643886    -0.684919     292.47
 H       4.846608    -1.836242    -1.752860      21.73
 C       6.563553    -0.056220    -1.548788      96.44
 O       7.209794     1.200094    -1.292421     277.29
 H       7.555314     1.303112    -0.331777      29.64
 H       6.387554    -0.083757    -2.697479      31.72
 H       7.195282    -0.969524    -1.370020      32.02
55
name= lig-ACN-Water-frame_227
 C      -4.115031    -0.014795    -3.153736      55.23
 H      -4.470469    -0.994662    -3.666402      27.32
 C      -3.515434     1.192642    -1.094912      64.65
 H      -3.249131     1.264482     0.000829      20.66
 C      -3.438733     2.323261    -1.889098       6.89
 O      -3.079385     3.671845    -1.345513     222.34
 C      -3.152808     3.754929     0.109248      99.24
 H      -2.322824     3.256361     0.566494      27.17
 H      -4.124075     3.332867     0.456044      26.43
 H      -3.289814     4.888472     0.609225      23.81
 C      -3.578091     2.281954    -3.315874      22.66
 O      -3.403912     3.467820    -4.067111     160.03
 H      -3.304737     4.208515    -3.466391      25.33
 C      -3.726433     1.054143    -3.905741      55.29
 H      -3.863438     0.850031    -5.021775      17.42
 C      -3.890508     0.022254    -1.734043      16.49
 C      -3.855030    -1.319774    -0.975164      98.98
 H      -4.471293    -2.067618    -1.485416      25.61
 O      -4.364920    -1.136412     0.355993     127.76
 H      -4.073897    -0.331376     0.865335      25.93
 C      -2.337915    -1.880199    -1.033520      81.85
 H      -1.950917    -2.031237    -2.090951      26.05
 C      -2.026635    -3.268130    -0.381317     119.81
 O      -2.924661    -4.222813    -1.021068     211.70
 H      -2.580048    -4.238557    -2.006373      28.87
 H      -2.211021    -3.359268     0.680580      26.55
 H      -0.986643    -3.339763    -0.553390      26.67
 C       1.780752    -0.759317    -2.112444      40.76
 H       2.184517    -1.033702    -3.102557      24.13
 C       1.835286     0.673495    -0.119807     114.29
 H       2.485294     1.453545     0.337138      15.74
 C       0.462531     0.358066     0.127642      17.03
 O      -0.370732     0.945226     1.061224     223.34
 C       0.136585     2.005587     1.832573     128.51
 H      -0.651188     2.302240     2.384694      26.75
 H       1.027182     1.803668     2.562952      24.83
 H       0.615241     2.871220     1.289580      24.85
 C      -0.212082    -0.665667    -0.635032      13.29
 O      -1.531518    -0.890455    -0.303369     165.77
 C       0.470476    -1.238832    -1.754555      59.25
 H      -0.037275    -1.902503    -2.438142      19.88
 C       2.550849     0.115561    -1.299265      82.70
 C       3.983624     0.647161    -1.557814      64.25
 H       4.276761     0.649565    -2.770168      19.79
 O       4.028071     2.078676    -1.284910     160.21
 H       4.403036     2.209340    -0.303234      26.32
 C       5.104779    -0.196798    -0.768151      91.78
 H       5.059704     0.078890     0.300757      27.56
 O       4.742319    -1.574304    -0.702021     313.57
 H       4.762138    -2.169433    -1.560626      28.33
 C       6.524924    -0.046206    -1.537216     102.77
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 O       7.306405     1.229627    -1.293221     229.10
 H       7.736704     0.998430    -0.433689      30.33
 H       6.342201    -0.043400    -2.642050      31.65
 H       7.183032    -0.839664    -1.216176      31.34
55
name= lig-ACN-Water-frame_228
 C      -4.086974    -0.064104    -3.115799      65.88
 H      -4.287974    -1.098357    -3.612881      27.16
 C      -3.537721     1.198264    -1.057172      51.56
 H      -3.173514     1.120902    -0.039527      22.52
 C      -3.378741     2.412088    -1.817762      14.64
 O      -3.042435     3.602431    -1.323594     220.66
 C      -3.150355     3.769007     0.073443     101.40
 H      -2.241506     3.418885     0.679170      26.01
 H      -4.069739     3.219581     0.451783      25.67
 H      -3.174938     4.939445     0.122173      24.26
 C      -3.532718     2.366943    -3.276932     -16.00
 O      -3.412311     3.498498    -4.074455     136.92
 H      -3.556969     4.342267    -3.531914      24.32
 C      -3.777703     1.068567    -3.993785      22.04
 H      -3.785654     1.154404    -5.135908      16.84
 C      -3.879114    -0.056671    -1.761768      10.91
 C      -3.855038    -1.328675    -0.999751      85.36
 H      -4.499866    -2.014954    -1.444727      25.44
 O      -4.408244    -1.145531     0.342892     165.32
 H      -3.753566    -0.479964     0.730203      27.46
 C      -2.373632    -1.879260    -1.017948      86.76
 H      -2.158080    -1.834511    -2.104991      28.12
 C      -2.066131    -3.247147    -0.414787     130.87
 O      -2.887867    -4.223516    -1.052593     242.11
 H      -2.636663    -4.290762    -1.992813      31.79
 H      -2.256427    -3.253939     0.655432      27.16
 H      -1.074894    -3.643849    -0.554610      26.74
 C       1.829774    -0.769147    -2.123150      47.91
 H       2.406158    -1.296704    -2.926853      17.53
 C       1.798232     0.749980    -0.210823      81.40
 H       2.129333     1.572936     0.577653      13.52
 C       0.489646     0.366590     0.147982      23.37
 O      -0.422152     1.002847     1.025560     204.99
 C       0.123624     2.073421     1.933246     113.10
 H      -0.565761     2.465020     2.490860      28.67
 H       0.872993     1.485724     2.536196      26.12
 H       0.452853     2.862903     1.164193      24.70
 C      -0.133957    -0.648594    -0.643972      11.23
 O      -1.511120    -0.874901    -0.325484     143.56
 C       0.503580    -1.125521    -1.834758      83.82
 H       0.130046    -1.915947    -2.374958      22.91
 C       2.431673     0.216868    -1.278548      33.00
 C       3.901431     0.645640    -1.505209      70.15
 H       4.140926     0.387218    -2.736227      22.66
 O       4.004628     2.101282    -1.323215     190.13
 H       4.080846     2.276956    -0.341919      25.72
 C       5.072113    -0.113073    -0.796689      89.35
 H       5.288922     0.251827     0.218797      27.88
 O       4.626498    -1.566947    -0.712841     312.75
 H       4.703252    -1.785475    -1.683707      27.24
 C       6.478266     0.025913    -1.460648     106.46
 O       7.365705     1.202542    -1.281558     245.64
 H       7.726495     1.218589    -0.372981      31.19
 H       6.374494    -0.142081    -2.529658      32.36
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 H       6.988554    -0.828367    -1.125294      32.72
55
name= lig-ACN-Water-frame_229
 C      -3.962910    -0.047093    -3.227579      12.63
 H      -4.198156    -1.018720    -3.766643      17.98
 C      -3.537885     1.191541    -1.145150      71.01
 H      -3.415774     1.282464    -0.111858      20.71
 C      -3.355399     2.330241    -1.884217      16.82
 O      -2.984608     3.582449    -1.334110     192.40
 C      -3.137690     3.829826     0.105842     108.54
 H      -2.200108     3.389028     0.642953      22.97
 H      -4.142926     3.486225     0.635091      24.13
 H      -3.218379     4.951393     0.254505      24.50
 C      -3.507637     2.347491    -3.288399      36.82
 O      -3.419723     3.517309    -4.053264     142.84
 H      -3.693145     4.383157    -3.549523      20.53
 C      -3.872915     1.204068    -3.872173      56.64
 H      -3.917821     1.164660    -4.969712      27.71
 C      -3.879653     0.002797    -1.768185      10.20
 C      -3.830381    -1.368710    -0.947931     106.82
 H      -4.332560    -2.139576    -1.392132      28.32
 O      -4.411450    -1.153148     0.352582     204.41
 H      -3.828368    -1.068114     1.116302      25.21
 C      -2.316313    -1.815511    -1.031362      96.59
 H      -2.068005    -1.861975    -2.082768      27.06
 C      -2.095386    -3.240227    -0.422118     109.56
 O      -2.937878    -4.286495    -1.106517     258.15
 H      -2.379298    -4.433144    -1.857333      32.03
 H      -2.456850    -3.191966     0.615608      26.48
 H      -0.998728    -3.352775    -0.435737      25.80
 C       1.892258    -0.717548    -2.068398      13.18
 H       2.485553    -1.296225    -2.825702      21.81
 C       1.650180     0.876213    -0.163144     103.64
 H       2.341656     1.704707     0.338284      18.31
 C       0.385744     0.384042     0.123895      17.41
 O      -0.449522     1.058519     1.034904     205.98
 C       0.132411     2.059241     1.956255     122.36
 H      -0.689125     2.320642     2.470422      26.24
 H       0.937859     1.748766     2.641078      26.42
 H       0.651242     2.938338     1.484424      24.47
 C      -0.193751    -0.619956    -0.718980      13.59
 O      -1.480121    -0.868858    -0.337921     185.42
 C       0.535789    -1.132242    -1.858384      42.12
 H      -0.044493    -1.744853    -2.464226      17.17
 C       2.449273     0.251529    -1.272403      55.53
 C       3.848929     0.696037    -1.519201      82.24
 H       3.978181     0.546051    -2.788744      24.58
 O       4.005330     2.123318    -1.357610     205.31
 H       3.998035     2.293584    -0.429402      31.15
 C       4.976697    -0.061997    -0.779084      97.14
 H       4.909681     0.157403     0.300376      26.82
 O       4.619488    -1.469386    -0.766970     331.28
 H       4.632627    -1.918471    -1.586851      30.78
 C       6.482680     0.016628    -1.437850      99.42
 O       7.344341     1.179510    -1.252720     257.50
 H       7.672765     1.119646    -0.330912      30.16
 H       6.406569    -0.039410    -2.486748      31.40
 H       6.956592    -0.813925    -1.044981      32.06
55
name= lig-ACN-Water-frame_230
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 C      -3.889376    -0.011581    -3.209202      59.77
 H      -4.083529    -0.850439    -3.862856      18.82
 C      -3.566437     1.182189    -1.166441      38.22
 H      -3.675267     1.163002    -0.109307      20.86
 C      -3.300678     2.382342    -1.898391      16.01
 O      -2.952922     3.609109    -1.312275     210.36
 C      -3.109728     3.884067     0.117092     110.99
 H      -2.260494     3.387442     0.841486      22.69
 H      -4.136152     3.352503     0.400432      23.62
 H      -3.053679     4.929687     0.224806      26.03
 C      -3.530944     2.437576    -3.277249       7.82
 O      -3.421710     3.538811    -4.039354      88.94
 H      -3.535733     4.386009    -3.517260      19.73
 C      -3.939830     1.202821    -3.927505      45.84
 H      -4.236305     1.239819    -4.936515      27.39
 C      -3.865601    -0.091570    -1.833488      29.33
 C      -3.766960    -1.291822    -0.978323      93.91
 H      -4.316198    -2.020510    -1.430049      28.32
 O      -4.412744    -1.189073     0.408742     167.27
 H      -3.646719    -1.278244     1.020328      26.31
 C      -2.301282    -1.831232    -1.054582      95.85
 H      -2.033087    -1.880527    -2.080592      27.89
 C      -2.177704    -3.223590    -0.395104     116.77
 O      -2.917358    -4.292280    -1.134421     221.13
 H      -2.380792    -4.654788    -1.923730      29.29
 H      -2.551921    -3.340517     0.647427      25.50
 H      -1.126941    -3.667457    -0.359368      23.71
 C       1.837522    -0.723052    -2.001697      67.35
 H       2.431886    -0.931369    -2.923414      17.94
 C       1.641657     0.915659    -0.220683      59.78
 H       1.848475     1.826794     0.409322      15.18
 C       0.327081     0.516507     0.063122      24.84
 O      -0.459949     1.078719     1.075363     228.57
 C       0.123965     2.015101     1.988788     124.86
 H      -0.649067     2.430379     2.652005      25.11
 H       0.795808     1.462998     2.579979      27.25
 H       0.448091     2.853251     1.392071      25.50
 C      -0.224014    -0.524866    -0.761613      22.86
 O      -1.509187    -0.893525    -0.329711     185.95
 C       0.523138    -1.158721    -1.817400      63.07
 H       0.208095    -1.788630    -2.653436      19.79
 C       2.419038     0.311350    -1.158635      45.78
 C       3.859500     0.792163    -1.600974      68.36
 H       4.157266     0.607935    -2.839009      21.66
 O       4.014242     2.208235    -1.375652     155.69
 H       4.406591     2.263915    -0.423194      24.12
 C       4.931871    -0.063750    -0.808601     108.26
 H       4.954825     0.278758     0.231141      25.62
 O       4.643443    -1.441394    -0.806721     315.55
 H       4.777782    -1.665349    -1.687728      33.90
 C       6.424282    -0.004038    -1.408918     108.94
 O       7.271978     1.178806    -1.212442     272.11
 H       7.708375     1.070081    -0.326817      28.67
 H       6.282558    -0.146578    -2.433102      34.82
 H       6.943185    -0.829693    -1.065338      32.70
55
name= lig-ACN-Water-frame_231
 C      -3.944736    -0.039617    -3.264978      78.10
 H      -4.013675    -0.984328    -3.688649      28.62
 C      -3.616568     1.216555    -1.155226      74.79
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 H      -3.432630     1.164974    -0.069411      20.33
 C      -3.302785     2.418586    -1.806441      -6.01
 O      -2.897749     3.662835    -1.295161     197.39
 C      -3.112335     3.855525     0.095934     108.46
 H      -2.258146     3.243102     0.745909      22.41
 H      -4.225188     3.712843     0.524284      24.65
 H      -3.042793     4.862581     0.207461      26.52
 C      -3.594449     2.426024    -3.280748      -6.63
 O      -3.408677     3.587770    -4.068246     108.30
 H      -3.618557     4.443726    -3.639422      19.69
 C      -3.917846     1.242767    -3.976834      75.49
 H      -4.056785     1.275331    -5.013040      22.13
 C      -3.783705     0.033738    -1.833394     -18.61
 C      -3.810331    -1.361153    -1.024186      73.59
 H      -4.424727    -2.051499    -1.499320      26.48
 O      -4.328539    -1.221547     0.366004     176.69
 H      -3.671125    -0.886602     1.069963      22.59
 C      -2.344612    -1.910636    -1.029916      91.52
 H      -2.064666    -1.932401    -2.063060      27.67
 C      -2.226806    -3.331964    -0.370098     109.60
 O      -2.946685    -4.277115    -1.135211     236.61
 H      -2.323332    -4.228050    -1.982227      27.73
 H      -2.710613    -3.118680     0.618145      24.23
 H      -1.074101    -3.476502    -0.224858      23.62
 C       1.834184    -0.638896    -1.945048      45.01
 H       2.281808    -1.144286    -2.829412      21.13
 C       1.640567     1.034265    -0.189006      92.61
 H       2.171111     1.815299     0.258515      18.67
 C       0.280146     0.606066    -0.017236       8.39
 O      -0.535910     1.040311     1.071200     191.34
 C       0.129984     1.976581     2.030340     112.60
 H      -0.729022     2.274796     2.768420      22.70
 H       0.920469     1.555267     2.533988      26.69
 H       0.597433     2.783747     1.585004      25.54
 C      -0.294735    -0.497033    -0.755188      14.35
 O      -1.521304    -0.900168    -0.303317     171.39
 C       0.492575    -1.114309    -1.734697      43.67
 H      -0.049223    -2.026029    -2.186879      14.70
 C       2.446276     0.351831    -1.238507      61.68
 C       3.847241     0.832117    -1.576873      75.93
 H       3.813688     0.646303    -2.834732      23.25
 O       4.064664     2.305862    -1.350091     134.07
 H       4.517450     2.414874    -0.368888      22.80
 C       4.992264    -0.002125    -0.859362      96.52
 H       5.020785     0.199816     0.223454      24.21
 O       4.643597    -1.488176    -0.850813     308.37
 H       4.611734    -1.913714    -1.682453      31.33
 C       6.372658    -0.001033    -1.419099     116.05
 O       7.166938     1.190622    -1.188914     249.83
 H       7.448972     1.228538    -0.209635      30.25
 H       6.391822    -0.117030    -2.455882      32.79
 H       6.804924    -0.841975    -0.962269      33.87
55
name= lig-ACN-Water-frame_232
 C      -3.997786     0.044130    -3.252961      93.64
 H      -4.129324    -0.816440    -3.826821      30.97
 C      -3.565209     1.305949    -1.086078      25.25
 H      -3.299917     1.328910     0.024520      21.06
 C      -3.411682     2.481167    -1.897056      10.86
 O      -2.889346     3.654831    -1.317241     197.84
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 C      -3.108869     3.897224     0.136139      95.70
 H      -2.429431     3.121735     0.829020      23.13
 H      -4.224083     3.547011     0.331073      24.17
 H      -2.782230     4.814692     0.390451      26.38
 C      -3.602171     2.462621    -3.262905       4.56
 O      -3.397900     3.541247    -4.078857     146.10
 H      -3.687795     4.406104    -3.717907      24.39
 C      -3.841887     1.221948    -3.948788      44.44
 H      -3.717502     1.243674    -5.017014      21.29
 C      -3.797651     0.042853    -1.844968     -51.79
 C      -3.811043    -1.347630    -1.038035      59.60
 H      -4.505140    -2.043798    -1.490370      23.50
 O      -4.261030    -1.248473     0.285041     153.16
 H      -3.778045    -0.480499     0.623674      27.77
 C      -2.374167    -1.957587    -1.020511      91.96
 H      -1.929878    -2.071013    -2.014920      25.97
 C      -2.255594    -3.276455    -0.269281     110.53
 O      -2.980276    -4.284266    -1.153339     193.79
 H      -2.704220    -4.256983    -2.071515      31.50
 H      -2.769283    -3.534756     0.706987      24.16
 H      -1.178359    -3.749156    -0.123044      23.10
 C       1.771331    -0.662255    -1.996367      31.28
 H       2.496426    -1.294692    -2.504861      15.26
 C       1.633973     1.084360    -0.237786      58.38
 H       1.989415     1.775936     0.383290      18.80
 C       0.268309     0.670648     0.016711      16.05
 O      -0.557077     1.061365     1.063833     207.95
 C       0.128022     1.893912     2.058970     115.78
 H      -0.743127     2.154714     2.885582      23.05
 H       0.839683     1.349574     2.512686      27.36
 H       0.335030     2.795978     1.591479      25.91
 C      -0.317350    -0.425485    -0.677657      13.65
 O      -1.586039    -0.937048    -0.262885     169.38
 C       0.478120    -1.065237    -1.630522      70.32
 H       0.275170    -2.109654    -2.139251      20.39
 C       2.379892     0.484185    -1.252722      34.99
 C       3.855280     0.889793    -1.531525      72.68
 H       4.180092     0.907705    -2.739873      21.26
 O       4.124739     2.305905    -1.276915     223.45
 H       4.343760     2.411843    -0.240010      22.64
 C       4.922992    -0.094119    -0.910071     119.49
 H       4.962605     0.249335     0.139373      24.61
 O       4.616967    -1.483838    -0.851475     367.45
 H       4.759935    -1.719604    -1.765462      27.70
 C       6.419301     0.006603    -1.493711     106.27
 O       7.077430     1.265570    -1.148261     254.27
 H       7.472771     1.063632    -0.196144      27.48
 H       6.405972    -0.158640    -2.560730      33.98
 H       7.020384    -0.773651    -1.037346      32.62
55
name= lig-ACN-Water-frame_233
 C      -3.998069     0.096192    -3.142405      43.47
 H      -4.276489    -0.824593    -3.653458      26.65
 C      -3.513819     1.275368    -1.206637      61.80
 H      -3.314591     1.319715    -0.084056      22.34
 C      -3.487122     2.519021    -1.831348      25.98
 O      -2.911167     3.684126    -1.319356     217.29
 C      -3.107623     3.848641     0.123340     108.29
 H      -2.502648     3.012230     0.795220      21.57
 H      -4.225253     3.980467     0.414019      24.63
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 H      -2.819526     4.844774     0.241431      24.96
 C      -3.592399     2.492365    -3.298887       1.26
 O      -3.374881     3.530513    -4.129570      68.42
 H      -3.356881     4.387619    -3.592898      23.08
 C      -3.749533     1.252952    -3.946027      46.65
 H      -3.825231     1.239993    -5.080109      17.69
 C      -3.873322     0.050971    -1.751007      53.57
 C      -3.776317    -1.287348    -1.138692      90.71
 H      -4.395246    -2.003973    -1.754827      25.69
 O      -4.250667    -1.235637     0.275884     198.92
 H      -3.980108    -0.459333     0.792909      27.33
 C      -2.318881    -1.925308    -0.961049      96.51
 H      -1.935183    -2.010774    -2.032770      25.87
 C      -2.337565    -3.371712    -0.265925     106.23
 O      -3.062302    -4.293266    -1.116248     253.29
 H      -2.419400    -4.251490    -1.820136      32.17
 H      -2.783336    -3.053038     0.731275      24.23
 H      -1.164291    -3.552253    -0.174880      22.45
 C       1.813305    -0.581837    -1.915547      33.25
 H       2.287526    -1.204390    -2.661971      20.60
 C       1.513628     1.136938    -0.255623      59.10
 H       1.925723     1.925174     0.279684      19.59
 C       0.236106     0.639958     0.077314      19.43
 O      -0.553654     1.137178     1.084375     233.14
 C       0.063979     1.836126     2.115523     126.17
 H      -0.705674     1.936386     3.076989      22.70
 H       0.914559     1.374292     2.423379      28.67
 H       0.446526     2.802210     1.855192      25.67
 C      -0.339027    -0.460348    -0.665925      11.27
 O      -1.601515    -0.921467    -0.194179     175.42
 C       0.501848    -1.103686    -1.589477      35.22
 H      -0.011965    -2.021931    -2.090195      14.98
 C       2.334781     0.523927    -1.338361      22.86
 C       3.863614     0.909016    -1.575911      84.96
 H       3.872011     0.780756    -2.794712      22.78
 O       4.171012     2.247725    -1.146428     194.15
 H       4.534840     2.326160    -0.180923      21.03
 C       4.957605    -0.109038    -0.875483      88.16
 H       5.088393     0.137399     0.202776      24.61
 O       4.557377    -1.494569    -0.879132     337.08
 H       4.657085    -2.022847    -1.694413      27.03
 C       6.404282     0.037214    -1.520053     101.74
 O       7.022866     1.317060    -1.126854     207.73
 H       7.525503     1.266107    -0.223840      27.44
 H       6.423209     0.128141    -2.624496      30.60
 H       7.018536    -0.854931    -1.223839      31.88
55
name= lig-ACN-Water-frame_234
 C      -4.018852     0.083958    -3.194912      55.59
 H      -4.272704    -0.917024    -3.673131      26.32
 C      -3.501277     1.306111    -1.133191      49.12
 H      -3.156660     1.266447    -0.079733      21.39
 C      -3.451687     2.510802    -1.907532      22.52
 O      -2.998862     3.702820    -1.296001     227.77
 C      -3.120265     3.900858     0.095135     109.16
 H      -2.572393     3.025709     0.702854      23.03
 H      -4.205426     3.856269     0.430816      26.00
 H      -2.462225     4.732668     0.445844      24.50
 C      -3.531396     2.484879    -3.298875       7.08
 O      -3.321075     3.585215    -4.176562      27.42
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 H      -3.434667     4.572626    -3.805111      23.18
 C      -3.761798     1.220280    -3.896337      44.59
 H      -3.880539     1.160360    -5.062930      18.16
 C      -3.877606     0.104798    -1.780115       7.68
 C      -3.726873    -1.265565    -1.026336      90.13
 H      -4.402439    -2.069777    -1.540055      24.33
 O      -4.340689    -1.257091     0.275407     188.02
 H      -3.723084    -0.604437     0.758283      27.36
 C      -2.322474    -1.848508    -0.985870      84.22
 H      -1.745217    -1.900212    -1.987086      24.22
 C      -2.375603    -3.263514    -0.290945     111.30
 O      -3.112920    -4.283134    -1.050049     186.79
 H      -2.656808    -4.703705    -1.860112      29.56
 H      -2.986152    -3.386753     0.660279      24.06
 H      -1.390477    -3.828545     0.007779      23.55
 C       1.761902    -0.625618    -1.908874      50.56
 H       2.304112    -0.876358    -2.807846      17.88
 C       1.473923     1.181818    -0.312141      46.79
 H       1.797471     2.150672     0.144289      18.02
 C       0.219141     0.597028     0.073738      16.97
 O      -0.616008     1.188116     1.083318     197.69
 C       0.116307     1.850371     2.271913      97.42
 H      -0.766089     1.735908     3.086905      23.03
 H       0.929624     1.269501     2.574242      27.07
 H       0.205573     2.926645     2.057907      23.66
 C      -0.320131    -0.533115    -0.577310      24.18
 O      -1.539674    -0.906036    -0.140251     189.80
 C       0.490556    -1.133121    -1.587961      45.36
 H       0.201575    -1.980030    -2.258881      20.42
 C       2.334626     0.573062    -1.246828      22.70
 C       3.818389     0.848861    -1.526520      83.63
 H       4.139392     0.933233    -2.665130      23.85
 O       4.195170     2.200106    -1.111033     187.44
 H       4.365307     2.225436    -0.137251      25.12
 C       4.968752    -0.117834    -0.916690      79.31
 H       4.976214     0.177493     0.151931      25.68
 O       4.497804    -1.533021    -0.873809     340.27
 H       4.622326    -1.784514    -1.851632      27.33
 C       6.345623     0.128079    -1.535471     101.20
 O       7.014514     1.319956    -1.088458     223.14
 H       7.299230     1.104499    -0.165534      28.57
 H       6.136259     0.141774    -2.662862      29.29
 H       7.013098    -0.783334    -1.314505      30.89
55
name= lig-ACN-Water-frame_235
 C      -4.036303     0.022787    -3.187522      43.29
 H      -4.198241    -0.900588    -3.876379      25.33
 C      -3.530245     1.344041    -1.107810      69.99
 H      -3.275998     1.385086    -0.079522      19.09
 C      -3.316026     2.508803    -1.870477       4.63
 O      -3.098808     3.764740    -1.349171     185.30
 C      -3.110161     3.876665     0.155954     103.54
 H      -2.668522     2.960161     0.685106      22.81
 H      -4.133751     4.092107     0.476473      26.18
 H      -2.645987     4.958149     0.286366      24.43
 C      -3.464120     2.511730    -3.365502      -0.36
 O      -3.254133     3.593912    -4.185961     114.05
 H      -3.771870     4.373755    -3.777782      20.79
 C      -3.840321     1.258935    -3.959717      20.06
 H      -3.788768     1.275703    -5.147000      21.19
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 C      -3.795428     0.056913    -1.772228     -13.62
 C      -3.796288    -1.232570    -0.982007      72.53
 H      -4.339327    -2.042174    -1.677348      24.64
 O      -4.409944    -1.216731     0.332978     193.21
 H      -3.834818    -1.029784     1.110076      23.82
 C      -2.315220    -1.827783    -0.938895      87.80
 H      -2.063854    -1.866356    -2.073034      24.96
 C      -2.398344    -3.236502    -0.289703      94.61
 O      -3.209039    -4.281658    -1.016079     206.34
 H      -2.552741    -4.418674    -1.783519      29.85
 H      -2.925148    -2.920248     0.642245      24.63
 H      -1.285620    -3.437783    -0.081481      24.48
 C       1.756349    -0.559507    -1.925735      47.22
 H       2.298033    -1.190033    -2.628837      21.57
 C       1.458885     1.219355    -0.304920      66.18
 H       1.704920     2.250772     0.220920      17.23
 C       0.243902     0.681668     0.111490      17.17
 O      -0.591601     1.238797     1.100418     222.20
 C       0.047616     1.804125     2.348428      91.88
 H      -0.624716     1.691939     3.258081      22.95
 H       1.048621     1.373881     2.515317      25.14
 H       0.328776     2.909785     2.196429      22.45
 C      -0.196983    -0.588770    -0.505984       6.27
 O      -1.523910    -0.963398    -0.086512     194.73
 C       0.487240    -1.155289    -1.620656      60.04
 H       0.100586    -1.996192    -2.130209      18.61
 C       2.305342     0.448230    -1.180887      38.28
 C       3.811561     0.854679    -1.458859      87.39
 H       3.786022     0.714739    -2.585462      24.13
 O       4.185410     2.192512    -1.122758     247.07
 H       4.170939     2.400342    -0.194919      25.16
 C       4.804502    -0.141267    -0.860915      93.11
 H       5.000000     0.085493     0.213969      24.41
 O       4.514123    -1.510411    -0.908224     296.07
 H       4.628711    -2.061842    -1.784876      26.08
 C       6.254018     0.132942    -1.582547      78.17
 O       7.006060     1.295335    -1.028412     155.86
 H       7.360409     1.163118    -0.139642      30.75
 H       6.302206     0.444292    -2.717962      28.09
 H       6.935691    -0.818600    -1.443810      30.70
55
name= lig-ACN-Water-frame_236
 C      -3.967424     0.129049    -3.180096      43.44
 H      -4.258578    -0.927818    -3.531747      24.48
 C      -3.532468     1.307656    -1.199225      59.55
 H      -3.699413     1.303760    -0.175799      21.71
 C      -3.268902     2.510980    -1.941988      11.66
 O      -3.170630     3.830890    -1.332913     176.12
 C      -3.152140     3.919380     0.120578     111.82
 H      -2.529497     3.172499     0.618404      24.17
 H      -4.125887     3.918683     0.554340      26.24
 H      -2.404072     4.878709     0.390757      23.20
 C      -3.436096     2.435872    -3.328144       8.78
 O      -3.210717     3.590605    -4.162327     141.50
 H      -3.354787     4.492827    -3.799494      16.80
 C      -3.862857     1.256943    -3.957556      68.57
 H      -4.059900     1.203841    -5.088946      24.23
 C      -3.767901     0.108531    -1.788704      11.99
 C      -3.808126    -1.211620    -0.963532      65.41
 H      -4.573632    -1.991764    -1.470331      21.42
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 O      -4.510525    -1.159785     0.394035     164.09
 H      -3.779910    -0.912921     0.986218      25.60
 C      -2.428892    -1.822462    -0.917405      74.27
 H      -1.886181    -1.786045    -1.914836      22.63
 C      -2.411013    -3.207755    -0.242070     124.18
 O      -3.209625    -4.191787    -0.973539     235.14
 H      -2.876301    -4.310547    -1.841675      33.55
 H      -2.769324    -3.285885     0.792669      25.01
 H      -1.457623    -3.754047    -0.209169      24.24
 C       1.754014    -0.646061    -1.926464      23.41
 H       2.484722    -1.135073    -2.590082      13.28
 C       1.486369     1.211191    -0.228604      37.53
 H       2.112138     2.177794     0.144652      14.60
 C       0.240314     0.673956     0.168068      19.69
 O      -0.552874     1.285032     1.147383     240.18
 C       0.039762     1.768293     2.335277      96.59
 H      -0.668149     1.501077     3.099808      23.34
 H       0.994895     1.149732     2.579737      22.72
 H       0.071543     2.938848     2.312567      21.51
 C      -0.235269    -0.553210    -0.458141      11.18
 O      -1.447355    -1.042192    -0.053167     231.47
 C       0.470376    -1.114039    -1.559497      58.35
 H       0.065872    -1.909031    -2.047284      20.14
 C       2.293922     0.465543    -1.128445      60.83
 C       3.675154     0.826503    -1.435197      87.29
 H       3.876892     0.832913    -2.495925      25.27
 O       4.136186     2.232912    -1.156026     185.63
 H       4.503946     2.261122    -0.216782      25.32
 C       4.852264    -0.114398    -0.848540     101.11
 H       4.882092     0.102887     0.245825      23.99
 O       4.519658    -1.556664    -0.937326     300.76
 H       4.651398    -1.755026    -1.947020      26.04
 C       6.186511     0.162204    -1.531866      83.44
 O       6.966174     1.259486    -0.991349     217.50
 H       7.222367     1.009384    -0.082104      30.28
 H       5.792526     0.370966    -2.649143      29.91
 H       6.725277    -0.898483    -1.557029      31.89
55
name= lig-ACN-Water-frame_237
 C      -3.932182     0.062279    -3.184131      40.33
 H      -4.338433    -0.747274    -3.836349      18.52
 C      -3.512009     1.414544    -1.162631      69.91
 H      -3.557847     1.549066    -0.102801      22.01
 C      -3.337281     2.561717    -1.900860      17.97
 O      -3.224749     3.814106    -1.358035     218.62
 C      -3.119476     3.931346     0.079112     108.26
 H      -2.525429     3.145699     0.414442      25.60
 H      -4.062846     3.846319     0.515552      26.19
 H      -2.840428     5.137848     0.359589      22.81
 C      -3.392484     2.518000    -3.370283      17.28
 O      -3.176676     3.550337    -4.139672     115.99
 H      -3.155698     4.262620    -3.489559      21.33
 C      -3.826414     1.278808    -3.941150      35.54
 H      -4.113879     1.268109    -4.985219      26.97
 C      -3.796760     0.112909    -1.789184      24.46
 C      -3.899700    -1.143151    -0.913041      82.33
 H      -4.446145    -1.972166    -1.592907      25.35
 O      -4.525574    -1.060505     0.372697     180.21
 H      -4.084878    -0.446313     1.039414      23.62
 C      -2.396790    -1.848338    -0.810762      82.23
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 H      -2.198236    -2.042533    -1.884655      28.51
 C      -2.359843    -3.295828    -0.210905     115.71
 O      -3.280354    -4.111958    -0.957678     191.08
 H      -2.871153    -4.121861    -1.877426      30.89
 H      -2.731575    -3.248654     0.781705      27.99
 H      -1.307278    -3.450506    -0.252754      27.75
 C       1.764810    -0.674318    -1.778620      69.18
 H       2.150070    -1.077434    -2.734134      18.24
 C       1.546341     1.101001    -0.141990      59.96
 H       1.805186     2.074266     0.491608      16.66
 C       0.265039     0.656074     0.221549      24.87
 O      -0.577030     1.287154     1.115411     231.92
 C       0.029212     1.734625     2.412040     102.72
 H      -0.587726     1.501279     3.179494      26.08
 H       1.150370     1.318435     2.597761      23.66
 H       0.249585     2.900312     2.409670      21.78
 C      -0.314258    -0.447299    -0.494956      13.51
 O      -1.465490    -1.102223     0.036609     177.90
 C       0.469091    -1.099515    -1.494588      59.44
 H       0.094971    -1.896549    -2.039635      21.70
 C       2.243074     0.476362    -1.156737      39.41
 C       3.741020     0.859018    -1.477975      86.37
 H       3.793257     0.701235    -2.505163      25.72
 O       4.059461     2.242361    -1.154362     208.64
 H       4.706367     2.327142    -0.340278      22.51
 C       4.787698    -0.124621    -0.796524      72.13
 H       4.902389     0.068145     0.306054      24.01
 O       4.538100    -1.548765    -0.966769     307.87
 H       4.572981    -1.955916    -1.885533      29.99
 C       6.106018     0.159788    -1.504839      92.61
 O       6.896218     1.212500    -0.992964     208.19
 H       7.298582     1.052020    -0.079573      28.55
 H       6.015270     0.566343    -2.650202      28.97
 H       6.857197    -0.761677    -1.535606      30.43
55
name= lig-ACN-Water-frame_238
 C      -3.958946     0.078410    -3.190989      42.13
 H      -4.164195    -0.890638    -3.587969      24.72
 C      -3.548344     1.403131    -1.121342      50.97
 H      -3.214402     1.418194    -0.046815      22.56
 C      -3.438305     2.584739    -1.923092      17.90
 O      -3.241703     3.859974    -1.417381     192.78
 C      -3.136730     3.926541     0.052782     116.47
 H      -2.291386     3.552883     0.508901      27.42
 H      -4.029968     3.693490     0.501433      26.90
 H      -2.826751     5.144573     0.112513      23.63
 C      -3.409199     2.451963    -3.290795      14.47
 O      -3.118042     3.617559    -4.146327     118.44
 H      -3.273434     4.596548    -3.834328      19.12
 C      -3.747585     1.269100    -3.930574      66.39
 H      -3.727809     1.319235    -4.957797      31.28
 C      -3.811314     0.167275    -1.727185     -11.10
 C      -3.820334    -1.141462    -0.878812      74.00
 H      -4.572810    -1.892463    -1.384687      22.78
 O      -4.570875    -0.934312     0.348997     160.66
 H      -4.001225    -0.257098     0.854090      27.55
 C      -2.419134    -1.850623    -0.719989     101.15
 H      -1.936366    -1.730232    -1.655526      28.62
 C      -2.340925    -3.274258    -0.155118     128.56
 O      -3.330058    -4.087636    -0.979804     158.85
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 H      -2.903743    -4.167663    -1.919356      29.38
 H      -2.601511    -3.317966     0.854768      28.37
 H      -1.499717    -3.854352    -0.240008      28.02
 C       1.715226    -0.627307    -1.746837      44.68
 H       2.335424    -1.177863    -2.492656      21.62
 C       1.554934     1.026155    -0.011483       8.05
 H       2.085142     1.892918     0.487076      19.50
 C       0.193863     0.602090     0.211227      -1.17
 O      -0.591750     1.297750     1.174781     202.67
 C       0.046528     1.746623     2.463226      91.40
 H      -0.529324     1.454421     3.228247      28.70
 H       1.083455     1.074371     2.506956      25.01
 H       0.081765     2.895155     2.344331      24.34
 C      -0.392206    -0.474840    -0.488420       7.26
 O      -1.506749    -1.069869     0.098397     187.69
 C       0.409579    -1.124876    -1.436514      52.44
 H      -0.020587    -2.014857    -1.915189      21.51
 C       2.351998     0.499995    -1.133769     -13.81
 C       3.742541     0.842240    -1.500556     103.46
 H       3.928139     0.803538    -2.487205      29.11
 O       4.003884     2.240433    -1.157040     218.61
 H       4.598302     2.358036    -0.409806      26.59
 C       4.739070    -0.157462    -0.845016      95.22
 H       4.758807     0.047953     0.268526      27.18
 O       4.508892    -1.543773    -0.944047     301.14
 H       4.735922    -1.838309    -1.852081      28.71
 C       6.155710     0.120799    -1.532488      72.50
 O       6.871598     1.276395    -0.967967     161.76
 H       7.186092     0.976437    -0.009437      23.05
 H       5.852327     0.303438    -2.697916      27.90
 H       6.622273    -0.960717    -1.453351      31.08
55
name= lig-ACN-Water-frame_239
 C      -3.961570     0.132190    -3.073423      73.89
 H      -4.006591    -0.771634    -3.571172      28.14
 C      -3.563487     1.402559    -1.120783      71.52
 H      -3.270608     1.487536    -0.012806      21.37
 C      -3.501408     2.581497    -1.868733       2.32
 O      -3.237708     3.882051    -1.420668     222.98
 C      -3.104217     4.053218    -0.010444     123.08
 H      -2.290304     3.499965     0.247139      26.80
 H      -3.915454     3.576148     0.514842      26.95
 H      -3.250559     5.224707     0.336049      24.38
 C      -3.467447     2.562886    -3.362857     -14.71
 O      -3.072949     3.603193    -4.139965      49.78
 H      -3.486740     4.455480    -3.697900      20.81
 C      -3.635086     1.227145    -3.957983      40.72
 H      -3.520140     1.031171    -4.957542      22.10
 C      -3.794054     0.146953    -1.734831       9.63
 C      -3.800918    -1.139976    -0.875415      83.07
 H      -4.311843    -1.969970    -1.479914      25.43
 O      -4.587953    -0.804761     0.359016     152.79
 H      -3.999303    -0.328022     1.008569      26.52
 C      -2.379006    -1.790263    -0.706460      93.03
 H      -2.080499    -1.963373    -1.688013      29.09
 C      -2.435641    -3.330132    -0.171968     120.68
 O      -3.353376    -4.062879    -0.981757     226.01
 H      -2.902056    -4.241435    -1.794655      33.51
 H      -2.817998    -3.420143     0.797665      27.40
 H      -1.449787    -3.537893    -0.242170      28.65
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 C       1.640896    -0.618005    -1.802012      32.03
 H       2.301410    -1.248288    -2.416176      18.50
 C       1.571747     0.998140     0.003358      66.24
 H       1.920181     1.729339     0.666348      21.26
 C       0.201507     0.658582     0.273251       6.30
 O      -0.596013     1.264419     1.244056     223.69
 C       0.045933     1.728090     2.427454     107.72
 H      -0.586880     1.453285     3.205303      26.52
 H       1.186106     1.318666     2.698039      23.45
 H       0.233139     2.839526     2.545228      23.60
 C      -0.379468    -0.527892    -0.368817      10.16
 O      -1.580026    -0.961077     0.190360     190.09
 C       0.403444    -1.137282    -1.432716      80.50
 H       0.232426    -2.167154    -1.927971      21.08
 C       2.242610     0.400939    -1.012233      32.94
 C       3.695901     0.825978    -1.508656     100.04
 H       3.642326     0.770573    -2.483770      27.48
 O       4.000789     2.225358    -1.161882     235.38
 H       4.454388     2.288013    -0.321555      24.93
 C       4.844525    -0.113213    -0.895337      94.60
 H       4.890066     0.163300     0.202688      23.40
 O       4.437475    -1.568818    -0.931438     326.93
 H       4.622532    -2.000798    -1.822960      28.49
 C       6.180066     0.070524    -1.476373     107.79
 O       6.844154     1.302777    -1.003576     190.66
 H       7.138230     1.248273     0.017181      25.26
 H       6.189208     0.278905    -2.658978      28.28
 H       7.033547    -0.665599    -1.284013      30.18
55
name= lig-ACN-Water-frame_240
 C      -3.863849     0.117567    -3.139112      52.85
 H      -4.138181    -0.774252    -3.613988      25.28
 C      -3.561259     1.484584    -1.114740      56.94
 H      -3.629034     1.642254    -0.013958      20.71
 C      -3.502942     2.626265    -1.967283      11.64
 O      -3.263812     3.918286    -1.439565     206.38
 C      -3.090752     4.100759    -0.014942     119.86
 H      -2.134004     3.962010     0.418623      26.11
 H      -3.950941     3.659536     0.551783      25.10
 H      -3.105159     5.282960     0.086495      25.44
 C      -3.513132     2.511511    -3.368826      12.21
 O      -3.068961     3.588207    -4.139154     110.19
 H      -3.056606     4.527601    -3.748928      19.35
 C      -3.574322     1.261760    -3.900605      63.85
 H      -3.541049     1.225199    -4.983084      21.41
 C      -3.762695     0.161775    -1.673404      -2.14
 C      -3.846786    -1.090302    -0.847727      97.82
 H      -4.537852    -1.813800    -1.303551      22.83
 O      -4.571020    -0.766739     0.353391     235.47
 H      -3.946058    -0.270120     0.937851      24.58
 C      -2.461389    -1.793684    -0.651621      95.76
 H      -1.954006    -1.671904    -1.522266      25.12
 C      -2.499113    -3.230056    -0.152423     128.89
 O      -3.353765    -4.083440    -1.028658     211.98
 H      -2.856493    -4.274399    -1.846373      30.52
 H      -2.916378    -3.255967     0.838794      25.60
 H      -1.642975    -3.768234    -0.104763      26.78
 C       1.605998    -0.659920    -1.787007      36.29
 H       1.974646    -0.985322    -2.766248      19.78
 C       1.521706     1.045237     0.067376      66.85
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 H       2.002841     1.782763     0.500106      20.63
 C       0.203348     0.606547     0.341061       9.92
 O      -0.567972     1.216252     1.274555     220.14
 C       0.061975     1.770349     2.506806      81.60
 H      -0.524351     1.494875     3.392286      23.41
 H       1.109521     1.182018     2.544813      21.94
 H       0.083514     2.825378     2.289337      23.35
 C      -0.265395    -0.529019    -0.279211      19.78
 O      -1.607671    -0.895858     0.190534     195.14
 C       0.337932    -1.157402    -1.355597      69.70
 H      -0.278808    -2.055648    -1.824120      13.82
 C       2.250760     0.326161    -1.021350      45.04
 C       3.633106     0.780333    -1.439798     100.57
 H       3.692138     0.727593    -2.416316      27.00
 O       4.007586     2.182763    -1.186837     199.55
 H       4.385161     2.292787    -0.224486      23.73
 C       4.816395    -0.171509    -0.908408      82.79
 H       4.985206     0.021424     0.195589      23.25
 O       4.402279    -1.525715    -0.896762     324.81
 H       4.499412    -1.964047    -1.851375      27.99
 C       6.372046     0.087828    -1.477325      83.10
 O       6.824804     1.389513    -1.051615     264.20
 H       7.162140     1.236973    -0.072918      26.97
 H       6.352943     0.005042    -2.638719      30.69
 H       6.759062    -0.877767    -1.045626      32.22
55
name= lig-ACN-Water-frame_241
 C      -3.723796     0.077227    -3.123691      42.76
 H      -3.957971    -0.909696    -3.531451      23.13
 C      -3.629250     1.529886    -1.165822      86.35
 H      -3.651967     1.638452    -0.117276      22.30
 C      -3.460135     2.680049    -1.899151      22.18
 O      -3.282334     3.950286    -1.467554     212.46
 C      -3.081979     4.215240    -0.034144     119.12
 H      -2.150731     3.745612     0.260394      24.58
 H      -3.882666     3.815392     0.713691      23.63
 H      -3.267487     5.338166    -0.018669      24.76
 C      -3.406037     2.548841    -3.337186       6.23
 O      -3.072025     3.553726    -4.199067     -15.02
 H      -3.394861     4.397233    -3.788125      19.93
 C      -3.616092     1.247997    -3.944466      36.48
 H      -3.618051     1.220690    -5.096317      23.83
 C      -3.726979     0.288748    -1.760971      45.31
 C      -3.930238    -1.035737    -0.814893      80.93
 H      -4.498406    -1.730999    -1.371782      27.24
 O      -4.569060    -0.763615     0.422850     199.32
 H      -3.934351    -0.325411     1.066222      22.40
 C      -2.482662    -1.692164    -0.679575      85.86
 H      -2.279091    -1.875438    -1.680339      27.88
 C      -2.567444    -3.194436    -0.090574     105.53
 O      -3.342815    -4.083364    -1.072613     172.66
 H      -2.716346    -4.060093    -1.914218      28.48
 H      -3.211421    -3.181998     0.799038      25.99
 H      -1.573356    -3.471921     0.086447      27.79
 C       1.534540    -0.700504    -1.744922      41.98
 H       1.962022    -0.965505    -2.709510      19.60
 C       1.589479     1.004296     0.011442      49.25
 H       1.904779     1.867393     0.370925      19.93
 C       0.302723     0.563958     0.448276      18.52
 O      -0.596059     1.194158     1.378228     226.54
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 C       0.086361     1.822392     2.507877     103.78
 H      -0.605528     1.574832     3.422547      22.73
 H       1.158111     1.477699     2.732422      25.51
 H       0.144716     2.877591     2.504546      24.51
 C      -0.378035    -0.592175    -0.201364      21.54
 O      -1.603701    -0.886476     0.176923     181.60
 C       0.303594    -1.172591    -1.299801      49.61
 H      -0.232978    -1.869158    -2.085292      19.05
 C       2.225664     0.363580    -1.016522      33.84
 C       3.702192     0.730263    -1.443371      91.48
 H       3.704302     0.621781    -2.426844      26.76
 O       3.988011     2.148381    -1.186388     178.65
 H       4.417968     2.248667    -0.286908      25.58
 C       4.827127    -0.160466    -0.857292      83.48
 H       4.883075     0.156919     0.222077      25.10
 O       4.408692    -1.527207    -0.870905     331.54
 H       4.473302    -1.871930    -1.917252      26.34
 C       6.317726     0.038545    -1.448099     113.14
 O       6.860806     1.435231    -1.080688     192.76
 H       7.211689     1.347717    -0.160482      28.59
 H       6.550454    -0.054227    -2.531383      32.02
 H       7.128759    -0.487293    -0.943833      30.98
55
name= lig-ACN-Water-frame_242
 C      -3.635774     0.119501    -3.157387      43.00
 H      -3.506152    -0.897937    -3.665675      22.27
 C      -3.696154     1.571732    -1.118952      55.05
 H      -3.719600     1.573921    -0.089455      22.27
 C      -3.391971     2.712685    -1.941914       3.16
 O      -3.312542     4.046625    -1.448353     214.82
 C      -3.084573     4.312530    -0.082895     126.85
 H      -2.080029     3.926761     0.285455      24.72
 H      -4.005102     3.856052     0.498559      23.71
 H      -2.918010     5.337101     0.119353      26.20
 C      -3.298604     2.486503    -3.382018      18.44
 O      -3.103299     3.551139    -4.269758     177.53
 H      -3.346176     4.429390    -3.899713      20.88
 C      -3.621401     1.253329    -3.953150      52.77
 H      -3.698269     1.140932    -5.139085      24.93
 C      -3.761315     0.237121    -1.730522      28.92
 C      -3.880755    -0.905177    -0.847815      92.97
 H      -4.513707    -1.590474    -1.284785      27.01
 O      -4.606898    -0.767698     0.503465     146.53
 H      -3.965635    -0.438295     1.243435      22.44
 C      -2.589975    -1.710647    -0.716425      88.47
 H      -1.990350    -1.671575    -1.591969      25.02
 C      -2.702510    -3.128062    -0.092384     120.00
 O      -3.239628    -4.014894    -1.079182     226.74
 H      -2.732981    -3.979838    -1.940994      29.16
 H      -3.335168    -3.247134     0.833439      24.58
 H      -1.732080    -3.497091     0.206226      26.36
 C       1.559444    -0.667051    -1.691536      36.51
 H       2.033466    -1.381757    -2.343983      21.02
 C       1.547331     0.990805     0.041807      61.81
 H       2.011282     1.824031     0.520018      20.40
 C       0.277224     0.476448     0.511099      11.57
 O      -0.512451     1.177615     1.449874     222.86
 C       0.082054     1.918158     2.572778     100.93
 H      -0.534723     1.640142     3.579163      21.85
 H       1.076075     1.525524     2.679015      26.90
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 H       0.077307     2.949001     2.292279      25.10
 C      -0.317686    -0.565870    -0.208829       9.35
 O      -1.727283    -0.923543     0.184187     165.46
 C       0.269071    -1.147285    -1.319054      65.76
 H      -0.197232    -2.014513    -1.882775      19.20
 C       2.278978     0.325546    -1.081918      40.99
 C       3.722768     0.739466    -1.524492      97.02
 H       3.868488     0.632415    -2.516236      27.74
 O       3.969641     2.131656    -1.188081     224.47
 H       4.486329     2.201370    -0.415085      27.96
 C       4.880134    -0.133803    -0.772845     104.98
 H       4.914174     0.049883     0.340090      26.19
 O       4.471579    -1.543698    -0.831444     319.65
 H       4.573876    -1.984203    -1.850498      23.08
 C       6.280892     0.094155    -1.330062     105.41
 O       6.874314     1.425466    -1.112728     235.06
 H       7.315723     1.383340    -0.248532      29.39
 H       6.098677    -0.038933    -2.365402      34.66
 H       6.753340    -0.803762    -0.970723      33.72
55
name= lig-ACN-Water-frame_243
 C      -3.605591     0.128739    -3.106907      32.02
 H      -3.574471    -0.960377    -3.539625      22.94
 C      -3.702181     1.603001    -1.158086     100.78
 H      -3.928984     1.816503    -0.146785      24.50
 C      -3.361154     2.705705    -1.977150     -22.34
 O      -3.325405     4.109419    -1.537783     167.80
 C      -3.061367     4.342020    -0.072583     122.35
 H      -2.185857     3.708780     0.376280      23.66
 H      -3.972019     4.203375     0.659673      25.84
 H      -3.035214     5.342661    -0.120534      28.05
 C      -3.304126     2.563070    -3.403059       0.01
 O      -3.129863     3.546473    -4.335517      51.46
 H      -3.007420     4.436155    -3.922746      19.59
 C      -3.511224     1.262000    -3.948247      22.58
 H      -3.535621     1.235569    -5.147281      24.84
 C      -3.766542     0.362282    -1.704445      23.80
 C      -3.958536    -0.975521    -0.791733      72.09
 H      -4.603737    -1.559989    -1.319040      27.89
 O      -4.592591    -0.746193     0.477257     172.39
 H      -3.962674    -0.247132     1.117823      24.99
 C      -2.569748    -1.691063    -0.657068      94.89
 H      -2.321595    -1.884100    -1.722214      28.37
 C      -2.772608    -3.080894    -0.110018     117.94
 O      -3.199451    -3.999411    -1.122090     228.83
 H      -2.585606    -3.917768    -1.833955      31.21
 H      -3.590845    -2.963598     0.665319      25.30
 H      -1.792284    -3.368590     0.369905      26.37
 C       1.634660    -0.790686    -1.715218      37.16
 H       2.225944    -1.313486    -2.463814      17.67
 C       1.562083     0.923731     0.045265      60.80
 H       2.041018     1.740502     0.695742      20.19
 C       0.270776     0.514577     0.493771      20.79
 O      -0.444782     1.124425     1.514380     219.66
 C       0.136743     1.984705     2.583181     107.32
 H      -0.613046     1.847464     3.562625      22.90
 H       1.113993     1.826220     2.861868      27.77
 H      -0.058897     3.051088     2.303608      24.13
 C      -0.491023    -0.562649    -0.206998      11.99
 O      -1.719390    -0.901954     0.226868     175.34
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 C       0.289134    -1.117829    -1.316614      73.97
 H      -0.046459    -2.081960    -1.644276      25.02
 C       2.258876     0.364168    -1.031327      22.38
 C       3.739035     0.729559    -1.452463      95.09
 H       3.816782     0.551281    -2.468494      25.90
 O       3.954600     2.167262    -1.224715     206.35
 H       4.531822     2.304213    -0.390690      24.97
 C       4.765565    -0.124994    -0.673563      92.46
 H       4.623697     0.222644     0.384209      26.51
 O       4.599618    -1.543233    -0.757937     341.74
 H       4.665970    -1.745916    -1.852076      23.95
 C       6.214511     0.099562    -1.312486     125.55
 O       6.900918     1.357603    -1.090228     241.20
 H       7.312184     1.255757    -0.173160      27.45
 H       6.202457     0.071879    -2.334945      34.54
 H       6.969389    -0.573275    -1.009006      32.32
55
name= lig-ACN-Water-frame_244
 C      -3.614414     0.185334    -3.033051      65.56
 H      -3.876852    -0.855327    -3.478559      27.30
 C      -3.687251     1.733057    -1.182796      59.20
 H      -3.917702     1.891778    -0.106393      26.66
 C      -3.402259     2.830947    -2.024019      15.06
 O      -3.313042     4.060921    -1.562450     198.42
 C      -3.102246     4.371504    -0.140219     119.82
 H      -2.136957     3.741498     0.173773      23.91
 H      -4.040224     4.075023     0.436813      25.30
 H      -2.834998     5.277430     0.013948      29.04
 C      -3.342646     2.587800    -3.433270      -4.87
 O      -3.118935     3.567588    -4.396174      36.79
 H      -3.402624     4.496429    -3.986265      23.29
 C      -3.343291     1.253392    -3.912281      57.36
 H      -3.203851     1.049424    -5.033118      18.42
 C      -3.769055     0.300870    -1.664230     -35.56
 C      -3.999098    -0.939596    -0.828927      81.34
 H      -4.539718    -1.710230    -1.236413      26.08
 O      -4.577013    -0.675313     0.455259     168.23
 H      -3.953345    -0.129295     0.977598      28.32
 C      -2.609165    -1.648848    -0.654158      75.91
 H      -1.962167    -1.602791    -1.592085      24.09
 C      -2.787752    -3.075340    -0.036795     107.44
 O      -3.220287    -4.008479    -1.127652     222.42
 H      -2.604909    -4.084940    -1.901877      28.32
 H      -3.667308    -3.194314     0.661398      23.50
 H      -1.888752    -3.456166     0.600524      24.71
 C       1.630481    -0.776302    -1.633011      76.73
 H       1.981720    -1.255684    -2.548366      15.90
 C       1.561313     0.867673     0.092709      64.28
 H       2.124897     1.789345     0.659026      18.41
 C       0.224500     0.563193     0.420904      18.97
 O      -0.409646     1.074321     1.618266     194.08
 C       0.155814     2.059895     2.540036     100.23
 H      -0.509256     1.797519     3.534503      23.14
 H       1.155062     1.853134     2.744885      28.40
 H       0.109798     3.152396     2.119100      23.69
 C      -0.403994    -0.460971    -0.289479      14.88
 O      -1.706170    -0.878423     0.239060     166.30
 C       0.322101    -1.203327    -1.263277      41.53
 H      -0.126964    -1.915368    -1.849345      18.39
 C       2.234620     0.285228    -1.024237      42.09
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 C       3.615701     0.731792    -1.338917      95.38
 H       3.799411     0.544359    -2.372657      25.58
 O       3.951218     2.205377    -1.270194     217.73
 H       4.487994     2.438399    -0.420846      24.99
 C       4.777771    -0.087011    -0.634457      85.65
 H       4.866010     0.086251     0.464738      26.00
 O       4.686309    -1.537481    -0.666610     287.94
 H       4.701686    -1.961794    -1.663010      25.49
 C       6.198039     0.096577    -1.299667      97.92
 O       6.928397     1.343618    -1.018704     257.97
 H       7.341663     1.363887    -0.033244      23.88
 H       6.014852    -0.052612    -2.277209      35.40
 H       6.618089    -0.784166    -0.922401      33.72
55
name= lig-ACN-Water-frame_245
 C      -3.642713     0.189928    -3.047212      54.58
 H      -3.687326    -0.819395    -3.545799      24.86
 C      -3.691700     1.678276    -1.168970      92.30
 H      -3.593469     1.931846    -0.056748      23.48
 C      -3.507032     2.774143    -2.075074      -3.92
 O      -3.293843     4.176391    -1.591276     195.55
 C      -3.127200     4.282288    -0.213578     127.28
 H      -2.250828     3.672178     0.317823      24.72
 H      -4.043529     4.021679     0.388966      25.94
 H      -3.081303     5.304857    -0.195622      28.31
 C      -3.294028     2.596366    -3.494137       8.24
 O      -3.129005     3.600919    -4.438478     107.11
 H      -3.214893     4.643262    -4.049239      20.52
 C      -3.225288     1.248723    -3.863082      48.40
 H      -3.034864     1.073635    -4.905838      22.36
 C      -3.810207     0.436206    -1.643890      15.39
 C      -3.913941    -0.871817    -0.832112      85.44
 H      -4.641818    -1.377811    -1.388992      26.14
 O      -4.592849    -0.568765     0.473272     187.09
 H      -3.925547    -0.263246     1.105103      28.48
 C      -2.571093    -1.650935    -0.599095      76.58
 H      -2.269392    -1.901151    -1.707629      24.68
 C      -2.818143    -3.108406    -0.041247     114.14
 O      -3.259921    -4.016494    -1.016559     171.74
 H      -2.613317    -3.881515    -1.835269      26.84
 H      -3.541004    -2.986033     0.785929      24.21
 H      -1.729914    -3.480668     0.303965      23.26
 C       1.566198    -0.785406    -1.649664      70.57
 H       2.175571    -1.287810    -2.430167      23.44
 C       1.544037     0.920451     0.141239      59.74
 H       2.195745     1.775199     0.783870      19.02
 C       0.232854     0.646024     0.490658      19.94
 O      -0.419642     1.011375     1.629518     211.58
 C       0.213540     2.060559     2.452563     100.84
 H      -0.320989     2.215256     3.491290      24.15
 H       1.241531     1.817163     2.640696      26.13
 H       0.039057     3.113317     1.891129      24.09
 C      -0.420773    -0.462416    -0.277819      11.74
 O      -1.657329    -0.806830     0.211669     173.84
 C       0.286733    -1.250006    -1.240007      54.26
 H      -0.188995    -1.988998    -1.776028      20.63
 C       2.210649     0.269434    -0.892646      31.63
 C       3.663010     0.734988    -1.329097      82.94
 H       3.661420     0.449526    -2.389391      25.04
 O       3.899627     2.197763    -1.278839     225.56
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 H       4.352145     2.350720    -0.462463      27.94
 C       4.867726    -0.080257    -0.584740     102.58
 H       4.901546     0.314119     0.455683      25.60
 O       4.676533    -1.556652    -0.574000     289.55
 H       4.638797    -1.781797    -1.545734      28.16
 C       6.204547     0.116602    -1.241332     118.49
 O       6.926920     1.324503    -0.992841     224.88
 H       7.387523     1.291106    -0.021728      22.66
 H       6.182493     0.178226    -2.252296      34.08
 H       6.896452    -0.637679    -1.008720      33.74
55
name= lig-ACN-Water-frame_246
 C      -3.603488     0.209762    -3.069766      74.11
 H      -3.483130    -0.830052    -3.326563      24.34
 C      -3.664043     1.784790    -1.167880      27.71
 H      -3.580906     1.808082    -0.028204      21.21
 C      -3.531159     2.860646    -2.075286      25.85
 O      -3.307181     4.127773    -1.717149     228.54
 C      -3.190851     4.260697    -0.179350     104.01
 H      -2.217124     3.692988     0.088979      23.62
 H      -4.073381     3.886934     0.281720      23.63
 H      -2.864479     5.290612     0.218265      24.13
 C      -3.259588     2.614012    -3.465544       1.53
 O      -3.129577     3.604877    -4.440369     143.36
 H      -3.165657     4.550778    -3.864383      22.49
 C      -3.195484     1.264606    -3.956305      53.77
 H      -2.914150     1.095079    -4.917497      24.79
 C      -3.799585     0.408524    -1.716578     -33.40
 C      -3.909547    -0.752400    -0.722719      93.16
 H      -4.451477    -1.592196    -1.135236      25.38
 O      -4.589993    -0.481492     0.490981     208.24
 H      -3.921113    -0.269445     1.226533      24.82
 C      -2.590198    -1.647899    -0.616986      72.04
 H      -2.034322    -1.713693    -1.646445      22.68
 C      -2.729899    -3.040177     0.035038     101.67
 O      -3.320052    -4.012670    -0.941010     193.55
 H      -2.833608    -4.019602    -1.839545      28.85
 H      -3.379726    -3.182526     0.901664      23.63
 H      -1.621454    -3.400200     0.419641      22.24
 C       1.581963    -0.754707    -1.587717      27.18
 H       2.139946    -1.380753    -2.328205      20.82
 C       1.557564     1.010344     0.190015     103.51
 H       2.151722     1.837287     0.897467      18.42
 C       0.237924     0.543269     0.516051       9.96
 O      -0.471053     1.011756     1.663158     210.69
 C       0.245575     2.074241     2.331211      93.22
 H      -0.333937     2.148787     3.268545      23.45
 H       1.365278     1.866188     2.547426      22.80
 H       0.253663     3.049593     1.644550      23.74
 C      -0.396252    -0.489553    -0.203384       6.48
 O      -1.714396    -0.783824     0.173723     183.95
 C       0.243758    -1.163444    -1.248421      79.02
 H      -0.079914    -2.155487    -1.492098      16.86
 C       2.248329     0.271589    -0.860383      84.51
 C       3.718136     0.649311    -1.324179      86.32
 H       3.903907     0.472318    -2.437690      24.75
 O       3.844994     2.134034    -1.250972     256.84
 H       4.356676     2.422942    -0.469895      24.96
 C       4.861652    -0.090634    -0.547472     119.71
 H       4.855306     0.186150     0.520838      22.70
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 O       4.615045    -1.508958    -0.499584     346.77
 H       4.608164    -1.839921    -1.347989      31.69
 C       6.342354     0.118620    -1.279758      99.21
 O       6.930489     1.403172    -0.988960     305.91
 H       7.349940     1.486423     0.017259      22.57
 H       6.017654     0.024684    -2.255758      36.75
 H       6.895200    -0.747268    -1.031491      33.50
55
name= lig-ACN-Water-frame_247
 C      -3.465949     0.202605    -3.117578      29.86
 H      -3.514452    -0.736225    -3.581859      24.16
 C      -3.678066     1.757699    -1.252300      78.58
 H      -3.888965     2.005054    -0.205902      23.15
 C      -3.451927     2.814949    -2.118620       7.40
 O      -3.328265     4.204690    -1.647248     203.36
 C      -3.185654     4.219185    -0.265978     120.58
 H      -2.445004     3.463549     0.105713      25.01
 H      -4.086262     3.996870     0.238043      25.37
 H      -2.990061     5.455447    -0.136293      23.76
 C      -3.295502     2.570077    -3.496393       8.44
 O      -3.105933     3.607194    -4.363815     -28.49
 H      -3.477460     4.557241    -4.072112      20.98
 C      -3.250263     1.275644    -3.999954      65.73
 H      -3.019179     1.157122    -4.981190      23.73
 C      -3.739699     0.462777    -1.686988     -23.45
 C      -3.954107    -0.823904    -0.744802      60.36
 H      -4.814040    -1.334754    -1.223461      23.45
 O      -4.563655    -0.385202     0.572096     192.83
 H      -3.883954    -0.105651     1.266200      25.89
 C      -2.599770    -1.532571    -0.590499      91.68
 H      -2.280143    -1.681241    -1.691323      23.94
 C      -2.653471    -3.015688     0.051761     105.57
 O      -3.309804    -3.950883    -0.879487     219.46
 H      -2.725598    -3.960499    -1.614927      32.16
 H      -3.268122    -2.891261     0.943246      24.42
 H      -1.514053    -3.435591     0.289255      23.26
 C       1.630033    -0.730627    -1.466485       4.04
 H       2.098089    -1.310105    -2.301290      13.82
 C       1.562540     0.920064     0.146963      76.13
 H       2.032846     1.891212     0.613275      13.33
 C       0.281533     0.484103     0.586602      36.22
 O      -0.469407     1.025846     1.620605     229.42
 C       0.220047     2.116452     2.282873     107.29
 H      -0.268187     2.465716     3.137098      25.05
 H       1.263771     1.632883     2.622181      23.49
 H       0.268587     3.026337     1.575630      24.05
 C      -0.426638    -0.526357    -0.146645      30.42
 O      -1.751464    -0.751069     0.231468     195.55
 C       0.295472    -1.105653    -1.228986     101.58
 H      -0.123953    -1.962639    -1.872846      17.76
 C       2.295849     0.314338    -0.888140      53.74
 C       3.717451     0.638380    -1.266182      90.83
 H       3.764068     0.221173    -2.366775      22.05
 O       3.844475     2.078918    -1.209003     221.32
 H       4.476981     2.239649    -0.384359      20.78
 C       4.931260    -0.091840    -0.541798      84.32
 H       5.042465     0.318672     0.466081      23.18
 O       4.545253    -1.495786    -0.447101     375.65
 H       4.543987    -1.781873    -1.369287      30.41
 C       6.297601     0.110535    -1.248643     121.34
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 O       6.935355     1.474118    -1.027775     249.75
 H       7.293303     1.456857    -0.025505      28.85
 H       6.431874     0.127254    -2.318478      32.79
 H       7.023443    -0.590314    -0.873327      31.73
55
name= lig-ACN-Water-frame_248
 C      -3.374142     0.168675    -3.097856      71.39
 H      -3.423352    -0.826176    -3.439299      25.92
 C      -3.738525     1.724296    -1.267646      60.68
 H      -4.093211     1.878816    -0.289420      27.47
 C      -3.379569     2.820330    -2.125278     -13.25
 O      -3.359741     4.171586    -1.688793     180.21
 C      -3.211998     4.252861    -0.236621     120.42
 H      -2.403438     3.687852     0.187172      26.14
 H      -4.117138     4.140256     0.267534      26.87
 H      -2.742602     5.419185     0.122149      24.10
 C      -3.325771     2.617320    -3.541250       8.05
 O      -3.097875     3.657215    -4.352590      87.19
 H      -3.189762     4.519292    -3.887907      20.98
 C      -3.317014     1.267590    -4.017038      57.27
 H      -3.386918     1.093813    -5.075393      20.93
 C      -3.651085     0.364802    -1.756525      12.10
 C      -4.033549    -0.723942    -0.729122      76.10
 H      -4.719767    -1.564436    -1.154106      25.43
 O      -4.521666    -0.325543     0.607338     189.23
 H      -3.701733    -0.106923     1.066924      29.51
 C      -2.640009    -1.579254    -0.579342      72.18
 H      -2.131353    -1.596423    -1.573189      26.74
 C      -2.632914    -2.912583     0.014308     128.85
 O      -3.251594    -3.856582    -0.814597     255.09
 H      -2.726255    -4.035877    -1.631402      29.82
 H      -3.119649    -3.029082     0.998767      26.47
 H      -1.441224    -3.196397     0.199475      24.50
 C       1.667876    -0.818343    -1.517267      45.52
 H       2.240798    -1.286491    -2.348456      20.99
 C       1.557768     0.905141     0.188319      69.68
 H       1.930048     1.819501     0.610888      17.92
 C       0.298542     0.446753     0.601250      19.32
 O      -0.458189     1.071891     1.587957     210.01
 C       0.185330     2.180681     2.293262     108.81
 H      -0.488056     2.460983     2.991072      26.56
 H       1.320281     1.946415     2.787530      23.90
 H       0.443330     2.956137     1.544428      25.55
 C      -0.420274    -0.539986    -0.134419      27.88
 O      -1.745559    -0.684671     0.301580     178.49
 C       0.294060    -1.137704    -1.183373      90.28
 H      -0.309713    -1.585002    -2.089815      18.48
 C       2.302322     0.270883    -0.820127      42.42
 C       3.731200     0.663709    -1.241672      82.18
 H       3.869092     0.514804    -2.417664      21.97
 O       3.928441     2.080754    -1.168808     249.09
 H       4.471329     2.391522    -0.358139      22.58
 C       4.913316    -0.068313    -0.542361     101.56
 H       5.013255     0.228875     0.495078      24.51
 O       4.538849    -1.489861    -0.425547     324.67
 H       4.445233    -1.874340    -1.424604      26.78
 C       6.345903     0.165027    -1.213275      97.24
 O       6.887092     1.466957    -1.028955     244.16
 H       7.212595     1.591170    -0.071071      28.41
 H       6.128323    -0.184850    -2.271702      32.43
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 H       6.944819    -0.607622    -0.689713      31.70
55
name= lig-ACN-Water-frame_249
 C      -3.371426     0.124750    -3.132324      48.71
 H      -3.120154    -0.846021    -3.558401      23.01
 C      -3.766813     1.707795    -1.302178     120.64
 H      -3.978694     1.803516    -0.285343      27.76
 C      -3.430468     2.767245    -2.095412       0.37
 O      -3.366862     4.105677    -1.711805     133.52
 C      -3.206425     4.324326    -0.152026     104.06
 H      -2.559946     3.570898     0.088032      25.68
 H      -4.135458     4.107821     0.313163      25.51
 H      -2.876979     5.593877    -0.024827      22.40
 C      -3.287341     2.597023    -3.499438      -3.91
 O      -3.110019     3.720505    -4.398902      95.95
 H      -3.070442     4.550193    -3.982314      21.72
 C      -3.387367     1.253717    -4.011564      29.86
 H      -3.378593     1.090352    -5.148268      23.87
 C      -3.675533     0.386939    -1.729461     -14.84
 C      -3.923441    -0.738325    -0.699170      78.89
 H      -4.837347    -1.396530    -1.111340      24.60
 O      -4.452751    -0.288543     0.549185     189.56
 H      -3.795684    -0.044821     1.248975      25.77
 C      -2.640129    -1.442101    -0.552869     101.45
 H      -2.271474    -1.581920    -1.553202      25.86
 C      -2.562020    -2.879871     0.090782     109.08
 O      -3.246777    -3.847913    -0.812426     201.86
 H      -2.671932    -3.854508    -1.695297      28.04
 H      -3.093043    -2.888104     1.088391      24.72
 H      -1.393279    -3.138409     0.234740      23.87
 C       1.629744    -0.847981    -1.528197      33.73
 H       2.022904    -1.404828    -2.378900      21.20
 C       1.601879     0.918041     0.259487      78.64
 H       2.076747     1.605004     0.797173      21.81
 C       0.294063     0.485383     0.610016      10.38
 O      -0.427725     1.130369     1.609939     210.19
 C       0.140322     2.266483     2.293992     105.49
 H      -0.620415     2.622167     2.922264      26.35
 H       1.025163     1.828101     3.068265      23.56
 H       0.305614     3.071465     1.625272      26.82
 C      -0.367613    -0.535195    -0.119378      18.64
 O      -1.754955    -0.672000     0.282958     195.07
 C       0.281219    -1.164368    -1.249282      70.85
 H      -0.275863    -2.074759    -1.788698      17.45
 C       2.315287     0.139940    -0.790010      56.34
 C       3.756616     0.720484    -1.240525      55.45
 H       3.802066     0.383508    -2.391896      21.92
 O       4.018623     2.175000    -1.135520     272.58
 H       4.334216     2.345795    -0.203391      24.70
 C       4.847744    -0.084862    -0.483868     112.27
 H       4.763387     0.261633     0.536394      24.63
 O       4.589698    -1.482139    -0.434012     315.51
 H       4.655713    -1.852938    -1.503790      26.09
 C       6.289789     0.086425    -1.125117     102.76
 O       6.833727     1.476710    -1.022707     222.19
 H       7.206157     1.573092    -0.131017      32.21
 H       6.373732     0.060829    -2.302262      31.80
 H       7.082327    -0.659426    -0.759532      31.41
55
name= lig-ACN-Water-frame_250
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 C      -3.446037     0.177082    -3.132386      59.11
 H      -3.286624    -0.871143    -3.514751      23.98
 C      -3.776437     1.683974    -1.244251      57.17
 H      -3.911990     1.948981    -0.203936      21.86
 C      -3.514604     2.799952    -2.133630      -9.55
 O      -3.361375     4.118124    -1.588482     209.96
 C      -3.240848     4.266753    -0.247474     130.95
 H      -2.468360     3.929251     0.346545      26.02
 H      -4.183715     4.229462     0.313541      25.85
 H      -2.935704     5.536100    -0.144109      23.68
 C      -3.274194     2.599703    -3.549576      13.25
 O      -3.136039     3.631865    -4.400303     160.80
 H      -3.423254     4.512937    -4.000626      19.58
 C      -3.370281     1.284668    -3.997128      51.44
 H      -3.070169     1.136688    -5.142533      22.99
 C      -3.726193     0.382109    -1.776682      45.44
 C      -3.853488    -0.717246    -0.697040      81.77
 H      -4.538029    -1.602625    -1.211563      25.82
 O      -4.447173    -0.241532     0.536080     203.67
 H      -3.621107     0.008721     1.077689      25.66
 C      -2.485928    -1.510078    -0.533567      90.33
 H      -2.089780    -1.566017    -1.507571      27.67
 C      -2.575247    -2.881885     0.103980     120.30
 O      -3.228310    -3.831268    -0.785450     235.09
 H      -2.758484    -3.779013    -1.658202      30.53
 H      -3.154692    -2.868069     1.099223      24.78
 H      -1.508633    -3.288313     0.328230      25.27
 C       1.583120    -0.825939    -1.516614      36.78
 H       2.183486    -1.325224    -2.255148      16.72
 C       1.705030     0.780416     0.271574      58.04
 H       2.205017     1.439627     0.768925      17.47
 C       0.329659     0.575507     0.601877      26.40
 O      -0.448277     1.154167     1.633742     223.16
 C       0.043229     2.339244     2.346405     105.59
 H      -0.770063     2.739113     2.984035      23.79
 H       1.081936     2.110580     3.011327      23.44
 H       0.504720     3.028246     1.666060      25.79
 C      -0.387455    -0.489814    -0.127881      28.87
 O      -1.668979    -0.613612     0.229631     200.73
 C       0.232508    -1.193719    -1.185588      90.56
 H      -0.060558    -2.228895    -1.590129      21.97
 C       2.318628     0.208677    -0.801910      51.18
 C       3.723042     0.699503    -1.218436      60.02
 H       3.859182     0.593154    -2.440175      19.82
 O       4.019771     2.169780    -1.152021     209.55
 H       4.446935     2.324217    -0.260389      25.44
 C       4.873443    -0.088693    -0.453317     109.39
 H       4.970972     0.162513     0.606488      26.09
 O       4.631682    -1.521084    -0.443874     356.31
 H       4.722207    -1.880258    -1.528803      23.00
 C       6.240295     0.110443    -1.072352      94.51
 O       6.801949     1.470580    -0.986433     230.57
 H       7.218405     1.487303    -0.100508      29.97
 H       6.038444    -0.280493    -2.187965      32.33
 H       6.958851    -0.632273    -0.509689      32.25
55
name= lig-ACN-Water-frame_251
 C      -3.560195     0.222739    -3.126659      44.92
 H      -3.651536    -0.831737    -3.574529      23.89
 C      -3.752537     1.759390    -1.279328      89.73
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 H      -3.906817     1.801223    -0.169661      25.36
 C      -3.568603     2.819552    -2.080716      33.03
 O      -3.354553     4.078619    -1.638206     197.64
 C      -3.280567     4.334608    -0.150763     109.52
 H      -2.503562     3.671137     0.090238      25.81
 H      -4.204159     3.887550     0.307287      24.72
 H      -3.178598     5.570935    -0.040332      23.13
 C      -3.388038     2.596283    -3.469207       1.36
 O      -3.153532     3.595986    -4.451269      94.69
 H      -3.310174     4.598420    -4.037705      20.84
 C      -3.246189     1.280252    -4.021624      39.18
 H      -3.067801     1.080321    -5.195926      19.90
 C      -3.767147     0.400293    -1.736068      -2.39
 C      -3.813413    -0.781399    -0.777949      66.28
 H      -4.668710    -1.638537    -0.999369      22.84
 O      -4.400161    -0.253027     0.508791     177.18
 H      -3.780954     0.120706     1.155383      27.61
 C      -2.403020    -1.537883    -0.567645      92.75
 H      -1.973847    -1.786095    -1.487617      25.13
 C      -2.584866    -2.933861     0.137205     112.78
 O      -3.247543    -3.815553    -0.773074     272.56
 H      -2.765766    -3.879870    -1.576965      32.29
 H      -3.308514    -2.872687     1.040331      24.06
 H      -1.584778    -3.269571     0.520963      24.73
 C       1.620743    -0.772271    -1.517959      87.41
 H       1.987365    -1.402253    -2.302557      20.05
 C       1.711991     0.803535     0.386825      63.77
 H       2.227864     1.480211     0.944896      18.07
 C       0.350397     0.586481     0.607051      18.07
 O      -0.444730     1.166374     1.643055     202.16
 C       0.039508     2.386377     2.346857      87.60
 H      -0.941845     2.765294     2.887189      23.07
 H       0.818973     2.075569     3.232007      22.32
 H       0.208511     3.192825     1.597039      24.52
 C      -0.305137    -0.356460    -0.151170      20.12
 O      -1.638077    -0.563799     0.243730     184.22
 C       0.357586    -1.192403    -1.050459      62.47
 H      -0.243299    -1.877519    -1.614141      17.50
 C       2.289580     0.263164    -0.900852      35.31
 C       3.742535     0.658718    -1.209537      69.14
 H       3.944021     0.188536    -2.356740      22.21
 O       3.946113     2.086601    -1.207696     219.55
 H       4.218011     2.405316    -0.331802      27.06
 C       4.846571    -0.116600    -0.428243      93.51
 H       4.734425     0.167641     0.637174      26.84
 O       4.655634    -1.552250    -0.418109     345.17
 H       4.640305    -1.899369    -1.503966      22.05
 C       6.244405     0.122412    -1.046217     103.63
 O       6.785967     1.435650    -0.983829     255.14
 H       7.180817     1.628192    -0.080809      28.28
 H       6.401630    -0.129295    -2.208874      32.44
 H       6.971890    -0.637702    -0.478627      31.60
55
name= lig-ACN-Water-frame_252
 C      -3.646467     0.197721    -3.160265      71.11
 H      -3.684398    -0.863011    -3.570829      24.20
 C      -3.760732     1.678678    -1.200036      78.13
 H      -3.803905     1.949540    -0.101740      25.01
 C      -3.564653     2.828017    -2.102909      -7.89
 O      -3.378256     4.191629    -1.669192     137.74
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 C      -3.320893     4.272844    -0.145615     118.29
 H      -2.399261     3.936463     0.372310      24.84
 H      -4.307088     3.963381     0.404282      24.05
 H      -3.152893     5.386651     0.143713      25.69
 C      -3.411774     2.604007    -3.547657      19.59
 O      -3.187589     3.614764    -4.458637     164.20
 H      -3.080745     4.554833    -4.020814      20.10
 C      -3.257638     1.284186    -3.930946      51.51
 H      -3.122301     1.201420    -5.086319      22.58
 C      -3.775133     0.413610    -1.767830      11.55
 C      -3.804255    -0.798044    -0.751776      91.15
 H      -4.546437    -1.544094    -1.376188      25.00
 O      -4.365877    -0.346393     0.477210     181.52
 H      -3.582179    -0.112432     1.005773      27.72
 C      -2.464122    -1.498453    -0.549571      91.37
 H      -2.057934    -1.541492    -1.546867      25.95
 C      -2.605065    -2.914093     0.198334     109.73
 O      -3.290115    -3.840056    -0.782698     232.72
 H      -2.576347    -3.938138    -1.505081      28.70
 H      -3.314521    -2.718238     1.069895      24.48
 H      -1.692970    -3.378244     0.520558      25.62
 C       1.688144    -0.754220    -1.525053      51.15
 H       2.143817    -1.110217    -2.441830      20.02
 C       1.738468     0.940094     0.325223      62.44
 H       2.364036     1.522571     1.038213      20.33
 C       0.389224     0.654648     0.719807      21.68
 O      -0.398571     1.190869     1.647097     230.05
 C      -0.050434     2.394071     2.326410      96.48
 H      -1.028238     2.730723     2.979043      22.04
 H       0.878771     2.241098     3.038040      24.21
 H       0.468820     3.182980     1.640914      24.49
 C      -0.316519    -0.340387    -0.104830      12.55
 O      -1.637630    -0.578608     0.224159     183.44
 C       0.437013    -1.126425    -1.033629      56.21
 H      -0.023968    -1.921541    -1.522479      21.40
 C       2.315416     0.321559    -0.785238      29.96
 C       3.718210     0.553153    -1.266733      69.21
 H       3.837288     0.323770    -2.511908      21.06
 O       3.876009     2.029431    -1.287372     213.74
 H       4.102894     2.193705    -0.337007      27.11
 C       4.815686    -0.163308    -0.411351     105.96
 H       4.836238     0.188476     0.660027      26.02
 O       4.637113    -1.572127    -0.368754     302.14
 H       4.788474    -1.926198    -1.409252      24.93
 C       6.301006     0.065244    -1.012079      87.05
 O       6.807023     1.477357    -1.003838     214.63
 H       7.162505     1.474501    -0.030409      27.22
 H       6.128367    -0.244432    -2.136007      33.91
 H       7.106459    -0.650532    -0.494249      31.80
55
name= lig-ACN-Water-frame_253
 C      -3.650822     0.166312    -3.122268      39.69
 H      -3.529119    -0.832855    -3.579623      24.60
 C      -3.722907     1.753797    -1.263067      55.13
 H      -3.739490     1.742389    -0.159203      27.93
 C      -3.539809     2.852711    -2.102223      27.11
 O      -3.424963     4.220638    -1.584551     181.36
 C      -3.322369     4.290203    -0.209293     122.32
 H      -2.542517     3.525228     0.145074      23.23
 H      -4.359978     3.891056     0.232492      23.12
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 H      -3.205802     5.357887    -0.050587      26.81
 C      -3.357203     2.647610    -3.479286      12.62
 O      -3.212774     3.655424    -4.438600     172.18
 H      -3.334558     4.513032    -4.067047      22.14
 C      -3.414455     1.290422    -3.999496      47.90
 H      -3.083765     1.047420    -5.022055      22.81
 C      -3.772757     0.365072    -1.738965     -24.62
 C      -3.862475    -0.771005    -0.822666      82.45
 H      -4.504666    -1.742996    -1.095036      23.98
 O      -4.372764    -0.477338     0.506575     149.63
 H      -3.651385    -0.313075     1.208159      25.24
 C      -2.486915    -1.502864    -0.562762      84.53
 H      -1.961848    -1.823001    -1.515818      24.40
 C      -2.687952    -2.859281     0.134452     114.27
 O      -3.299320    -3.826864    -0.734615     245.44
 H      -2.683597    -4.003555    -1.552489      29.89
 H      -3.307774    -2.913879     1.050317      25.10
 H      -1.727676    -3.098909     0.440783      28.29
 C       1.697260    -0.656597    -1.434714      36.90
 H       2.239742    -1.214163    -2.221004      23.45
 C       1.734177     1.061826     0.304345      94.24
 H       2.352016     1.935564     0.859480      23.62
 C       0.430483     0.642618     0.644644      10.43
 O      -0.412806     1.221218     1.706314     182.80
 C      -0.019119     2.454315     2.346200      95.47
 H      -1.026110     2.894064     2.942826      22.54
 H       0.776244     2.260833     3.129979      24.79
 H       0.104217     3.277509     1.490364      23.58
 C      -0.239894    -0.415466    -0.043057      11.48
 O      -1.638276    -0.584471     0.248805     161.38
 C       0.368418    -1.076108    -1.098576      65.50
 H      -0.025085    -1.989562    -1.457057      19.41
 C       2.392136     0.268688    -0.720543      47.59
 C       3.726240     0.593612    -1.275532      75.38
 H       3.759519     0.034937    -2.442311      20.88
 O       3.869511     1.993412    -1.345079     254.25
 H       4.377264     2.402598    -0.547210      21.94
 C       4.913526    -0.165433    -0.436420     114.44
 H       4.725204     0.169815     0.638498      24.16
 O       4.602501    -1.618516    -0.324798     304.41
 H       4.568661    -2.007949    -1.292806      27.41
 C       6.274851     0.061485    -1.022006     102.31
 O       6.826506     1.441218    -1.020810     194.96
 H       7.297201     1.679570    -0.120803      27.13
 H       6.345769    -0.272077    -2.120426      32.74
 H       7.013883    -0.645341    -0.428099      29.81
55
name= lig-ACN-Water-frame_254
 C      -3.587412     0.216406    -3.150393      62.20
 H      -3.604504    -0.797286    -3.472008      26.82
 C      -3.684920     1.729497    -1.284282      66.97
 H      -3.853965     1.951707    -0.267054      22.79
 C      -3.495795     2.889189    -2.073791      18.44
 O      -3.482824     4.160395    -1.651323     204.68
 C      -3.348315     4.289658    -0.176124     119.60
 H      -2.500783     3.588078     0.234622      24.00
 H      -4.358206     4.129086     0.441620      25.13
 H      -2.960678     5.168525     0.157727      28.57
 C      -3.369471     2.631841    -3.494473       8.26
 O      -3.230555     3.691949    -4.392435     176.55
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 H      -3.316158     4.574608    -4.057072      21.58
 C      -3.539869     1.305916    -4.012183      54.47
 H      -3.474786     1.255178    -5.043908      23.21
 C      -3.790532     0.454966    -1.758559      45.05
 C      -3.841803    -0.858904    -0.764960      82.39
 H      -4.629161    -1.392209    -1.399740      25.55
 O      -4.448447    -0.565512     0.572731     178.59
 H      -3.704645    -0.310320     1.175042      25.35
 C      -2.478685    -1.503331    -0.602128      82.18
 H      -2.003828    -1.586337    -1.686846      22.69
 C      -2.687764    -2.836937     0.141354     120.69
 O      -3.326015    -3.831600    -0.721216     286.52
 H      -2.838669    -3.796725    -1.537883      33.32
 H      -3.360770    -2.636647     0.948563      25.81
 H      -1.799330    -3.239919     0.440382      28.70
 C       1.644169    -0.732067    -1.369350      35.42
 H       2.157465    -1.416333    -2.089912      22.89
 C       1.700813     1.085132     0.289214      60.90
 H       2.023253     2.225561     0.690903      17.78
 C       0.371731     0.679213     0.660366      17.61
 O      -0.388335     1.217001     1.706504     205.18
 C      -0.006299     2.545401     2.347509      92.80
 H      -1.002379     2.762694     3.029312      21.53
 H       0.899993     2.517824     2.936453      25.32
 H       0.329036     3.387876     1.540207      23.47
 C      -0.294435    -0.445735     0.000420      15.04
 O      -1.619642    -0.615454     0.293852     167.41
 C       0.341094    -1.066919    -1.134358      74.44
 H      -0.184012    -1.720687    -1.876774      19.48
 C       2.402222     0.316058    -0.666710      46.00
 C       3.837576     0.572543    -1.190493      73.13
 H       3.901436     0.210606    -2.441631      22.25
 O       3.941107     2.051467    -1.412072     222.29
 H       4.591909     2.276367    -0.692257      24.23
 C       4.870922    -0.161194    -0.456186     111.86
 H       5.054829     0.233309     0.599892      22.21
 O       4.578661    -1.605461    -0.331466     342.18
 H       4.557737    -1.949470    -1.213131      31.02
 C       6.355680     0.040708    -1.052335      96.68
 O       6.842688     1.401724    -1.016549     203.54
 H       7.109240     1.461617    -0.035933      28.91
 H       6.410652    -0.294501    -2.107216      33.24
 H       7.063760    -0.605090    -0.403043      31.47
55
name= lig-ACN-Water-frame_255
 C      -3.609402     0.242802    -3.145126      44.56
 H      -3.706650    -0.672629    -3.638960      24.16
 C      -3.701260     1.767326    -1.177092      55.67
 H      -3.891869     1.878303    -0.167144      24.53
 C      -3.473304     2.781682    -2.144391      -1.69
 O      -3.520703     4.181342    -1.627751     143.41
 C      -3.315510     4.299363    -0.135018     108.52
 H      -2.656758     3.438043     0.349923      24.13
 H      -4.386623     4.265920     0.351136      25.14
 H      -2.999967     5.191400    -0.136448      29.23
 C      -3.451608     2.667877    -3.528922      23.32
 O      -3.243945     3.692525    -4.371615      86.49
 H      -3.128429     4.571614    -3.866802      19.28
 C      -3.574115     1.396954    -4.045641      50.28
 H      -3.820763     1.235796    -4.999892      22.20
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 C      -3.717630     0.409601    -1.721050     -24.30
 C      -3.870208    -0.731170    -0.762305      71.37
 H      -4.344322    -1.678822    -1.091108      24.34
 O      -4.481837    -0.588422     0.550012     168.76
 H      -3.886848    -0.160722     1.174059      27.47
 C      -2.468811    -1.493922    -0.578333      71.81
 H      -1.941109    -1.515907    -1.673701      21.83
 C      -2.632793    -2.873094     0.155783     116.07
 O      -3.380936    -3.823315    -0.733533     268.11
 H      -2.940464    -3.850984    -1.593735      30.81
 H      -3.253337    -2.689398     0.985738      26.52
 H      -1.761589    -3.210332     0.609709      28.11
 C       1.735812    -0.805761    -1.298502      24.09
 H       2.284730    -1.197990    -2.185443      12.19
 C       1.583628     1.055998     0.250836      57.07
 H       2.226703     2.011581     0.753936      20.47
 C       0.333431     0.656150     0.681311      17.03
 O      -0.344404     1.299644     1.733767     225.82
 C       0.033343     2.540675     2.292230     108.65
 H      -0.807102     2.905076     3.054553      23.58
 H       0.914719     2.402000     2.830152      26.34
 H      -0.027271     3.381521     1.417454      24.30
 C      -0.357918    -0.384044    -0.057942      17.67
 O      -1.684886    -0.686445     0.323814     194.02
 C       0.307534    -1.014788    -1.075569      81.22
 H      -0.282884    -1.680040    -1.821691      20.14
 C       2.331075     0.304372    -0.725675      51.26
 C       3.755568     0.626341    -1.207101      51.25
 H       3.833263     0.038238    -2.375652      23.22
 O       4.083462     2.093529    -1.405721     215.38
 H       4.610208     2.394954    -0.671553      26.92
 C       5.018777    -0.179055    -0.395602      76.68
 H       4.896742     0.122781     0.683870      24.79
 O       4.565074    -1.532884    -0.381728     405.98
 H       4.757808    -1.937730    -1.198895      34.58
 C       6.392567    -0.053755    -1.077023     109.57
 O       6.867875     1.383653    -0.949249     219.72
 H       7.100208     1.545677    -0.012354      29.70
 H       6.351299    -0.334240    -2.112266      34.96
 H       7.106705    -0.740009    -0.560297      32.18
55
name= lig-ACN-Water-frame_256
 C      -3.707956     0.303969    -3.121862      54.95
 H      -3.753484    -0.705965    -3.453591      25.68
 C      -3.706943     1.700027    -1.212870      85.13
 H      -3.768745     1.885765    -0.170247      24.82
 C      -3.546460     2.858943    -2.003841       7.18
 O      -3.501863     4.110543    -1.565544     230.79
 C      -3.328501     4.350967    -0.212641     127.83
 H      -2.571762     3.553786     0.220216      23.83
 H      -4.321360     4.273670     0.386321      25.21
 H      -2.891717     5.130244     0.088429      29.02
 C      -3.496311     2.681841    -3.486201      -3.12
 O      -3.243988     3.724503    -4.400996      80.50
 H      -3.521074     4.705353    -4.047113      18.18
 C      -3.625711     1.319616    -4.041810      48.53
 H      -3.527049     1.199119    -5.077892      21.61
 C      -3.670406     0.434201    -1.700500      23.23
 C      -3.807746    -0.816709    -0.770181      89.22
 H      -4.559192    -1.307193    -1.350684      24.84
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 O      -4.492604    -0.488987     0.490511     159.37
 H      -3.880744    -0.029350     1.157811      23.91
 C      -2.515668    -1.504042    -0.496672      93.84
 H      -1.995745    -1.798016    -1.546436      21.46
 C      -2.654637    -2.910975     0.117059     123.96
 O      -3.408868    -3.792997    -0.711284     249.43
 H      -2.844238    -3.962028    -1.574141      28.75
 H      -3.206583    -2.936942     1.006444      24.78
 H      -1.665686    -3.275005     0.135818      24.92
 C       1.690852    -0.806362    -1.335165      23.98
 H       2.087303    -1.524603    -2.076045      15.96
 C       1.596937     1.022127     0.222909      76.55
 H       2.142856     1.822856     0.958088      20.19
 C       0.273566     0.676096     0.679667      17.36
 O      -0.384720     1.279732     1.738285     221.63
 C       0.093268     2.585874     2.238154     106.70
 H      -0.637829     2.770969     3.071854      23.58
 H       1.075703     2.661161     2.577366      25.47
 H       0.113739     3.426840     1.373417      23.73
 C      -0.414632    -0.286287    -0.055478      14.76
 O      -1.678599    -0.690239     0.359063     197.98
 C       0.381410    -1.032937    -1.050943      60.84
 H      -0.055750    -2.019167    -1.481374      16.52
 C       2.343398     0.330363    -0.755151      49.66
 C       3.805890     0.707748    -1.199239      62.52
 H       3.845561     0.313563    -2.447873      17.98
 O       4.168870     2.077915    -1.349779     243.55
 H       4.599011     2.264231    -0.449790      21.79
 C       4.972822    -0.160527    -0.400176      94.65
 H       5.175822     0.212249     0.623696      20.93
 O       4.587330    -1.537494    -0.421376     353.34
 H       4.684085    -1.867290    -1.384405      26.56
 C       6.412437    -0.024882    -1.044660     124.40
 O       6.915102     1.315995    -0.865907     288.01
 H       7.183160     1.461964     0.067368      32.36
 H       6.315563    -0.105561    -2.081549      37.04
 H       7.123220    -0.740368    -0.692094      33.54
55
name= lig-ACN-Water-frame_257
 C      -3.783580     0.199005    -3.096962      48.96
 H      -3.783718    -0.813024    -3.540377      23.77
 C      -3.667679     1.751636    -1.165486      54.51
 H      -3.660810     1.817886    -0.050278      22.50
 C      -3.657827     2.835337    -2.070403      27.68
 O      -3.476466     4.173794    -1.568396     212.63
 C      -3.290298     4.350232    -0.120544     112.97
 H      -2.564175     3.587035     0.332827      23.25
 H      -4.293471     4.254191     0.406989      23.93
 H      -3.038661     5.291625    -0.209652      27.03
 C      -3.530165     2.675122    -3.455495      18.18
 O      -3.287744     3.669737    -4.397147     120.14
 H      -3.261761     4.683984    -3.918256      19.46
 C      -3.626297     1.408842    -3.941014      68.48
 H      -3.399178     1.244195    -5.023271      21.74
 C      -3.688317     0.418210    -1.725641     -12.64
 C      -3.854487    -0.786907    -0.807574      87.37
 H      -4.359166    -1.623891    -1.191985      26.03
 O      -4.512470    -0.362898     0.422448     164.37
 H      -3.732691    -0.220041     1.078249      23.04
 C      -2.540226    -1.600167    -0.501028      63.66
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 H      -1.950677    -1.541331    -1.502424      22.00
 C      -2.662345    -2.971943     0.152782     116.19
 O      -3.474088    -3.802229    -0.737433     256.93
 H      -2.936948    -3.906481    -1.576167      29.84
 H      -3.005172    -2.885801     1.175658      25.38
 H      -1.609089    -3.359312     0.429709      24.01
 C       1.675890    -0.726921    -1.403198      47.35
 H       2.328489    -1.420926    -1.912810      13.29
 C       1.656246     1.019173     0.288205      62.48
 H       2.200227     1.906957     0.756031      17.28
 C       0.293699     0.759703     0.599468       3.96
 O      -0.394151     1.272857     1.737951     196.72
 C       0.134338     2.626954     2.187334     101.15
 H      -0.392453     2.948134     3.046847      24.93
 H       1.158101     2.416859     2.408192      23.99
 H      -0.126880     3.370967     1.330136      23.59
 C      -0.387028    -0.340150    -0.112916       8.95
 O      -1.647701    -0.661442     0.384175     163.39
 C       0.324482    -1.113732    -0.945059      57.94
 H      -0.126503    -2.066077    -1.287535      19.16
 C       2.397923     0.347486    -0.788988      38.33
 C       3.896635     0.661925    -1.194174      56.16
 H       4.011462     0.290768    -2.441998      19.02
 O       4.213653     2.105390    -1.203429     234.90
 H       4.600777     2.481278    -0.324649      24.42
 C       4.912401    -0.130136    -0.480274     115.28
 H       4.754685     0.101991     0.567657      24.73
 O       4.612257    -1.564490    -0.423528     348.20
 H       4.585086    -1.981033    -1.410986      22.68
 C       6.356363     0.044335    -1.061300     117.02
 O       7.029589     1.301437    -0.761978     250.89
 H       7.162429     1.393049     0.256371      28.07
 H       6.402967    -0.096653    -2.105739      34.42
 H       6.852603    -0.728035    -0.609292      33.93
55
name= lig-ACN-Water-frame_258
 C      -3.773225     0.238670    -3.136135      59.16
 H      -3.892613    -0.751919    -3.679085      24.24
 C      -3.642851     1.715013    -1.206814      53.03
 H      -3.617504     1.954298    -0.078982      21.43
 C      -3.671083     2.895356    -2.010451      16.57
 O      -3.469360     4.197373    -1.585675     237.81
 C      -3.280371     4.385406    -0.088017     124.09
 H      -2.424684     3.855480     0.359598      25.36
 H      -4.209445     4.154830     0.425814      27.05
 H      -3.014070     5.389848     0.231805      27.39
 C      -3.579410     2.679552    -3.426917       6.62
 O      -3.336098     3.630711    -4.367380      76.86
 H      -3.182828     4.619139    -3.920002      19.30
 C      -3.604943     1.302886    -3.910604      60.63
 H      -3.694467     1.265028    -5.080618      21.73
 C      -3.797882     0.387458    -1.716455      24.78
 C      -3.881832    -0.807473    -0.766600      93.87
 H      -4.570178    -1.421471    -1.238321      28.19
 O      -4.525440    -0.275234     0.400869     205.00
 H      -4.018414    -0.359785     1.225544      25.90
 C      -2.456911    -1.501282    -0.504983      82.63
 H      -2.053964    -1.821752    -1.472701      25.44
 C      -2.672995    -2.994563     0.214092      94.87
 O      -3.528912    -3.826323    -0.731634     194.72
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 H      -3.135234    -3.778696    -1.578704      33.79
 H      -3.468596    -2.937073     0.977359      24.81
 H      -1.653196    -3.544692     0.408709      23.64
 C       1.679713    -0.712962    -1.374847      49.61
 H       2.030462    -1.170875    -2.280040      21.37
 C       1.747591     1.071795     0.266471      61.92
 H       2.232239     1.847371     0.755393      17.78
 C       0.351995     0.771963     0.545460       3.40
 O      -0.357834     1.331244     1.689137     205.90
 C       0.133349     2.579603     2.125257     129.34
 H      -0.329663     2.808520     2.992876      26.86
 H       1.238203     2.694362     2.326739      24.85
 H       0.016580     3.404059     1.332562      25.59
 C      -0.333443    -0.336311    -0.016175      -7.02
 O      -1.648418    -0.685631     0.341429     164.56
 C       0.436836    -1.186343    -0.981380      39.83
 H      -0.001110    -1.986678    -1.495616      18.79
 C       2.359428     0.359592    -0.779822      35.61
 C       3.804286     0.681254    -1.255115      71.33
 H       3.913978     0.517705    -2.534840      21.97
 O       4.219858     2.139914    -1.052526     199.92
 H       4.406419     2.178470    -0.089697      27.83
 C       4.893887    -0.169452    -0.448382      96.53
 H       4.985720     0.218946     0.547334      28.02
 O       4.625779    -1.573528    -0.393536     273.07
 H       4.732674    -1.888991    -1.399362      24.78
 C       6.335963     0.064559    -0.995150     102.20
 O       7.135183     1.301756    -0.695788     161.97
 H       7.321967     1.499150     0.341916      25.26
 H       6.270558     0.060555    -2.076994      31.45
 H       6.888495    -0.729985    -0.687145      33.93
55
name= lig-ACN-Water-frame_259
 C      -3.772826     0.211367    -3.099632      29.65
 H      -3.892659    -0.885484    -3.426107      23.10
 C      -3.685541     1.708617    -1.224586      78.85
 H      -3.587371     1.643537    -0.086482      24.31
 C      -3.574631     2.867646    -1.978723     -18.29
 O      -3.454870     4.241257    -1.498690     212.54
 C      -3.270299     4.400695    -0.127390     127.04
 H      -2.409994     3.827608     0.096014      26.76
 H      -4.039093     3.963424     0.381810      27.33
 H      -3.213825     5.565234    -0.066677      25.61
 C      -3.590991     2.621474    -3.413697      -1.52
 O      -3.384763     3.656407    -4.348326      38.37
 H      -3.578527     4.580809    -3.984821      21.14
 C      -3.639538     1.371366    -4.001485      53.11
 H      -3.689416     1.184406    -5.176048      19.23
 C      -3.831311     0.415573    -1.729209      13.88
 C      -3.863345    -0.769370    -0.740554      83.15
 H      -4.393532    -1.586611    -1.085721      27.31
 O      -4.582470    -0.279218     0.476150     187.75
 H      -3.923118    -0.179318     1.201449      25.03
 C      -2.499036    -1.566625    -0.473094      85.54
 H      -2.021248    -1.574968    -1.400867      25.69
 C      -2.841024    -2.923265     0.146596     114.59
 O      -3.533114    -3.823697    -0.708392     228.53
 H      -3.074900    -3.760851    -1.611395      28.79
 H      -3.242256    -2.778790     1.204854      25.30
 H      -1.804849    -3.415041     0.511327      24.39
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 C       1.746268    -0.733180    -1.425786      46.22
 H       2.139820    -1.101373    -2.355618      17.96
 C       1.708806     1.109989     0.228431      66.72
 H       2.195773     1.746584     0.767401      23.01
 C       0.410790     0.711508     0.630266       9.88
 O      -0.291798     1.352939     1.553743     210.81
 C       0.154186     2.650079     2.105543     107.85
 H      -0.447899     2.713808     2.923922      27.21
 H       1.263114     2.487261     2.392090      24.21
 H      -0.145816     3.430890     1.401465      26.36
 C      -0.213245    -0.464389    -0.024554      16.54
 O      -1.582324    -0.661392     0.305720     170.75
 C       0.444690    -1.119090    -0.973061      43.24
 H      -0.016703    -1.839353    -1.534282      22.56
 C       2.383058     0.384019    -0.792712      32.35
 C       3.747091     0.792597    -1.200090      73.94
 H       3.840595     0.634749    -2.471687      20.21
 O       4.150638     2.106330    -0.929837     251.52
 H       4.215872     2.356017     0.005070      24.90
 C       4.900009    -0.130007    -0.388982      68.88
 H       4.699189     0.137104     0.633695      24.28
 O       4.644142    -1.552291    -0.318340     285.91
 H       4.520341    -1.981640    -1.265442      26.72
 C       6.420520     0.088815    -0.970845      98.54
 O       7.167365     1.273412    -0.683939     215.84
 H       7.248172     1.387104     0.360810      29.67
 H       6.314966     0.174826    -2.077901      29.48
 H       6.977668    -0.772577    -0.768195      32.00
55
name= lig-ACN-Water-frame_260
 C      -3.793298     0.220269    -3.154156      71.07
 H      -3.723162    -0.778481    -3.664940      25.52
 C      -3.710617     1.740878    -1.109458      51.23
 H      -3.716722     1.981334    -0.030444      24.30
 C      -3.492848     2.841793    -2.024631      -2.01
 O      -3.471561     4.162269    -1.573828     198.95
 C      -3.215740     4.372210    -0.125450     124.66
 H      -2.308207     4.172715     0.289372      27.18
 H      -3.959811     4.035667     0.450177      27.75
 H      -3.248481     5.585085     0.083026      25.15
 C      -3.539944     2.674735    -3.445983      11.88
 O      -3.469877     3.723289    -4.326536     177.24
 H      -3.334836     4.514309    -3.811567      23.24
 C      -3.716848     1.322445    -3.964611      52.52
 H      -3.570026     1.327885    -5.109838      20.68
 C      -3.782470     0.416822    -1.721211      -2.85
 C      -3.888696    -0.717421    -0.694333      79.90
 H      -4.554572    -1.387684    -1.147254      25.93
 O      -4.601261    -0.379170     0.544399     174.91
 H      -3.990489     0.017636     1.250050      23.35
 C      -2.564041    -1.461709    -0.509695      80.53
 H      -2.207867    -1.743702    -1.421852      27.14
 C      -2.837091    -2.851585     0.196429      91.58
 O      -3.564304    -3.793275    -0.712164     158.23
 H      -2.941883    -3.932232    -1.546590      28.44
 H      -3.689069    -2.738960     0.967059      22.99
 H      -1.776456    -3.319179     0.428918      23.70
 C       1.814897    -0.686928    -1.476427      17.39
 H       2.437822    -1.341608    -2.082897      18.72
 C       1.705838     1.070975     0.193145      64.76
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 H       2.033608     1.938146     0.546436      20.88
 C       0.459874     0.575672     0.653891      13.27
 O      -0.328935     1.387805     1.502865     205.09
 C       0.129051     2.659391     2.105808     113.77
 H      -0.468515     2.912240     2.979747      25.62
 H       1.249476     2.723237     2.454942      24.73
 H       0.094480     3.441068     1.411006      28.27
 C      -0.188469    -0.480629     0.039905       6.39
 O      -1.541123    -0.664286     0.349728     143.69
 C       0.501571    -1.136149    -1.111510      71.57
 H      -0.027055    -1.938790    -1.565113      18.89
 C       2.391067     0.382757    -0.816972      38.96
 C       3.869173     0.750420    -1.079459      81.37
 H       4.084681     0.629458    -2.323773      20.46
 O       4.037381     2.200260    -0.870423     280.84
 H       4.408276     2.289723     0.057618      23.72
 C       4.912738    -0.075488    -0.364866     114.61
 H       4.980940     0.311041     0.658187      24.60
 O       4.641682    -1.520612    -0.241944     309.40
 H       4.714096    -1.859005    -1.268025      23.08
 C       6.389856     0.072366    -0.995761      92.90
 O       7.164067     1.274507    -0.667017     214.23
 H       7.238264     1.513889     0.298780      32.27
 H       6.351907    -0.031245    -2.138445      29.86
 H       6.926808    -0.790315    -0.599344      31.83
55
name= lig-ACN-Water-frame_261
 C      -3.785120     0.266772    -3.066901      42.42
 H      -3.787873    -0.745450    -3.458465      26.48
 C      -3.676183     1.758489    -1.195204     108.46
 H      -3.830837     1.864138    -0.167305      26.33
 C      -3.505538     2.802249    -2.011914      12.81
 O      -3.435616     4.102114    -1.599834     202.45
 C      -3.173424     4.402231    -0.152855     115.66
 H      -2.283144     4.012624    -0.001782      28.55
 H      -3.844311     3.860290     0.399478      27.80
 H      -3.299569     5.650247    -0.117642      24.01
 C      -3.522949     2.654575    -3.447001      14.77
 O      -3.530015     3.792955    -4.293947     124.12
 H      -3.350579     4.653567    -3.891328      21.44
 C      -3.709250     1.397240    -3.963932      61.51
 H      -3.835527     1.180877    -5.015205      23.38
 C      -3.759432     0.485263    -1.642637     -19.39
 C      -3.960911    -0.682155    -0.687971      78.22
 H      -4.540763    -1.442307    -1.188999      24.01
 O      -4.630428    -0.482443     0.557890     220.36
 H      -4.005733    -0.306023     1.357650      23.04
 C      -2.550073    -1.430033    -0.479682      78.74
 H      -2.069042    -1.359309    -1.424522      25.05
 C      -2.850620    -2.807677     0.204343      98.64
 O      -3.556738    -3.726642    -0.724115     247.85
 H      -2.948689    -3.960289    -1.428628      30.18
 H      -3.507885    -2.652970     1.162177      22.50
 H      -1.948472    -3.282214     0.769318      24.50
 C       1.827599    -0.744017    -1.464508      10.67
 H       2.335458    -1.351557    -2.264016      18.75
 C       1.719681     1.032284     0.192703      57.77
 H       2.091569     2.004493     0.498053      17.64
 C       0.443015     0.632857     0.678351     -11.75
 O      -0.394957     1.399051     1.519945     194.13
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 C       0.123649     2.633610     2.064313     104.47
 H      -0.698424     2.827683     2.828742      24.02
 H       1.147291     2.383840     2.553269      24.08
 H       0.065332     3.318600     1.308272      27.89
 C      -0.191120    -0.541706    -0.086271      -6.45
 O      -1.583641    -0.718227     0.390166     147.40
 C       0.508679    -1.130639    -1.129391      50.75
 H       0.189356    -1.994723    -1.760787      20.88
 C       2.493866     0.349484    -0.820313      36.33
 C       3.908868     0.770581    -1.068285      67.89
 H       4.176039     0.510610    -2.268303      18.55
 O       3.966583     2.260592    -0.889327     289.31
 H       4.336835     2.475959     0.013182      23.93
 C       5.052517    -0.050912    -0.275928     100.29
 H       5.189498     0.226573     0.797438      24.02
 O       4.634713    -1.442787    -0.216993     305.09
 H       4.774915    -1.921160    -1.125513      26.13
 C       6.356994     0.032752    -0.944893     105.28
 O       7.124532     1.293216    -0.689370     193.66
 H       7.048748     1.450625     0.250792      35.14
 H       6.341130    -0.044905    -2.107943      29.96
 H       6.964183    -0.847289    -0.530731      31.17
55
name= lig-ACN-Water-frame_262
 C      -3.766699     0.318306    -2.994893      59.16
 H      -4.015210    -0.648510    -3.340309      25.08
 C      -3.645774     1.767775    -1.116496      61.17
 H      -3.634996     1.961080    -0.095139      22.98
 C      -3.520207     2.885946    -2.067356       5.49
 O      -3.398993     4.180849    -1.586859     257.94
 C      -3.105374     4.348017    -0.288506     132.43
 H      -2.201222     4.161652     0.048077      28.23
 H      -3.809340     4.026635     0.466142      25.94
 H      -3.094144     5.594359    -0.073035      24.70
 C      -3.542745     2.723324    -3.452405       6.02
 O      -3.563857     3.801071    -4.274827      87.60
 H      -3.837981     4.584741    -3.713615      20.88
 C      -3.687697     1.364949    -3.952999      52.84
 H      -3.923382     1.253396    -4.951631      21.23
 C      -3.814385     0.447158    -1.622927      30.03
 C      -3.908727    -0.751140    -0.700634      70.26
 H      -4.424642    -1.565860    -1.250173      27.13
 O      -4.722001    -0.540061     0.546094     167.00
 H      -4.092167    -0.396488     1.314780      24.22
 C      -2.513528    -1.458774    -0.442436      88.81
 H      -2.130127    -1.773592    -1.441707      27.68
 C      -2.852541    -2.798301     0.198708     110.39
 O      -3.532399    -3.649419    -0.688530     202.19
 H      -2.961509    -3.709865    -1.458717      32.11
 H      -3.601663    -2.591478     1.044696      24.90
 H      -1.856109    -3.276663     0.416347      26.06
 C       1.875417    -0.785636    -1.432079      57.73
 H       2.308053    -1.124089    -2.423913      18.51
 C       1.717762     1.001569     0.217690      62.00
 H       2.264825     1.821640     0.865285      18.24
 C       0.359154     0.654425     0.516146      12.10
 O      -0.440158     1.287285     1.493964     213.34
 C       0.079857     2.560647     2.022501     114.38
 H      -0.640799     3.094915     2.850227      23.05
 H       1.068429     2.470944     2.578914      24.87
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 H       0.282186     3.228688     1.319933      28.60
 C      -0.278767    -0.429203    -0.069024       7.23
 O      -1.568043    -0.757981     0.407913     192.59
 C       0.486407    -1.159676    -1.094870      53.82
 H      -0.176893    -1.919612    -1.670097      17.40
 C       2.476426     0.266478    -0.725419      43.75
 C       3.934427     0.840013    -1.065631      79.58
 H       4.184902     0.669950    -2.258857      20.98
 O       3.975145     2.237779    -0.978846     304.49
 H       4.304905     2.476897    -0.052183      23.60
 C       5.044746    -0.038044    -0.190937      86.17
 H       4.942558     0.359103     0.870003      23.92
 O       4.638935    -1.401949    -0.194708     313.81
 H       4.562528    -1.623881    -1.111768      33.87
 C       6.512110     0.033766    -0.901763      97.56
 O       7.050729     1.295068    -0.699466     215.62
 H       7.100822     1.578430     0.246457      33.11
 H       6.225560    -0.083451    -2.042138      31.35
 H       7.255639    -0.854421    -0.630509      30.25
55
name= lig-ACN-Water-frame_263
 C      -3.829362     0.274665    -3.047809      16.46
 H      -3.940618    -0.641934    -3.567464      24.51
 C      -3.610128     1.846658    -1.078590      90.28
 H      -3.390663     2.024878    -0.039767      27.21
 C      -3.527108     2.871969    -1.977125       0.11
 O      -3.386425     4.256066    -1.693899     173.56
 C      -2.971402     4.437207    -0.194453     109.68
 H      -2.152927     3.887265    -0.078540      29.62
 H      -3.829474     3.939775     0.305648      25.47
 H      -2.947368     5.654507    -0.103361      24.52
 C      -3.614698     2.703461    -3.423866       4.18
 O      -3.610209     3.800367    -4.300556      52.21
 H      -3.582104     4.808879    -3.870340      19.72
 C      -3.680094     1.384832    -3.900942      56.69
 H      -3.636944     1.219149    -4.934107      21.94
 C      -3.826068     0.500683    -1.544509     -61.19
 C      -3.856605    -0.802223    -0.684936      70.61
 H      -4.474667    -1.535347    -1.320042      21.24
 O      -4.784268    -0.596042     0.458277     179.17
 H      -4.350987    -0.241344     1.240379      29.25
 C      -2.520060    -1.494194    -0.416390      80.53
 H      -1.917239    -1.550615    -1.425325      25.10
 C      -2.769036    -2.836495     0.278118     111.63
 O      -3.558503    -3.634477    -0.708663     145.50
 H      -3.133097    -3.628889    -1.666699      26.98
 H      -3.351924    -2.849736     1.229809      25.70
 H      -1.811952    -3.273050     0.610217      26.95
 C       1.748214    -0.792853    -1.380325      48.53
 H       2.307265    -1.411111    -2.147619      21.26
 C       1.687992     0.938862     0.284461      57.10
 H       2.208583     1.763805     1.052758      16.77
 C       0.301962     0.732271     0.458952       7.08
 O      -0.458547     1.223847     1.495368     223.10
 C       0.065041     2.487287     1.990855     101.33
 H      -0.929818     2.897195     2.588378      22.95
 H       0.927156     2.279613     2.617514      25.14
 H       0.226340     3.021013     1.124999      27.61
 C      -0.309139    -0.426511    -0.165828       5.12
 O      -1.537263    -0.762749     0.400852     167.95
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 C       0.459377    -1.132478    -1.041414      47.93
 H       0.064818    -2.018322    -1.685077      22.32
 C       2.476747     0.265344    -0.667090      37.28
 C       3.915185     0.729321    -1.042763      76.16
 H       4.045606     0.376942    -2.183415      21.26
 O       4.051246     2.249830    -1.027323     217.61
 H       4.522588     2.511785    -0.129409      22.88
 C       5.020509    -0.001852    -0.247573      98.12
 H       5.183585     0.312231     0.851325      23.80
 O       4.630234    -1.413256    -0.181080     287.48
 H       4.409708    -1.722944    -1.070099      29.27
 C       6.490014     0.035680    -0.831147      93.61
 O       7.069155     1.403337    -0.693341     174.41
 H       7.107971     1.540028     0.336648      29.18
 H       6.507460    -0.135255    -1.987281      29.18
 H       7.218024    -0.782238    -0.287340      29.42
55
name= lig-ACN-Water-frame_264
 C      -3.887746     0.310642    -2.957207      73.96
 H      -3.788737    -0.747332    -3.156231      28.69
 C      -3.569783     1.790178    -1.074234      63.17
 H      -3.418434     1.858597     0.047878      27.30
 C      -3.550818     2.986419    -1.988958      -0.81
 O      -3.323615     4.306907    -1.643944     203.17
 C      -2.915733     4.497765    -0.267846     117.39
 H      -2.022559     3.993672    -0.021990      28.24
 H      -3.689012     4.276176     0.593447      25.76
 H      -2.583713     5.558595    -0.002201      26.35
 C      -3.685253     2.729865    -3.368956      13.51
 O      -3.629649     3.739730    -4.304614     122.81
 H      -3.452576     4.658029    -3.760083      20.68
 C      -3.695808     1.407594    -3.887711      34.55
 H      -3.527568     1.298299    -4.976636      18.49
 C      -3.763746     0.510855    -1.627335      -5.76
 C      -3.916064    -0.696843    -0.708012      69.18
 H      -4.292878    -1.593346    -1.365382      23.76
 O      -4.818229    -0.661479     0.380783     160.81
 H      -4.303479    -0.320498     1.161410      27.65
 C      -2.477409    -1.510544    -0.352797      79.81
 H      -2.180205    -1.715958    -1.452321      27.76
 C      -2.693293    -2.955861     0.269651     114.09
 O      -3.579902    -3.659047    -0.690827     181.40
 H      -2.968515    -3.578841    -1.501716      29.10
 H      -3.260331    -2.734659     1.165149      26.13
 H      -1.778981    -3.500129     0.367928      27.22
 C       1.770906    -0.758774    -1.316482      53.72
 H       2.346571    -1.455847    -1.967238      21.28
 C       1.668001     0.941652     0.351919      67.75
 H       2.256790     1.882318     0.944762      16.65
 C       0.288932     0.651709     0.493717      18.98
 O      -0.485707     1.194116     1.502188     232.23
 C      -0.007950     2.439969     1.968165     119.13
 H      -0.825606     3.042564     2.624507      24.85
 H       0.798722     2.402554     2.663712      27.34
 H       0.327466     3.177775     1.241173      28.47
 C      -0.342134    -0.386435    -0.192475       7.10
 O      -1.558146    -0.731848     0.402145     176.60
 C       0.397166    -1.183562    -1.109399      82.39
 H       0.026023    -2.188294    -1.456811      17.46
 C       2.405239     0.287605    -0.657066      44.23
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 C       3.867934     0.678018    -1.022720      94.83
 H       4.007934     0.418265    -2.140036      26.43
 O       4.138346     2.160258    -1.074547     194.78
 H       4.352429     2.488141    -0.103716      26.04
 C       5.024544    -0.055678    -0.309982      85.20
 H       4.925624     0.347284     0.772336      25.24
 O       4.626561    -1.452299    -0.159716     292.85
 H       4.715140    -1.852304    -1.140755      26.93
 C       6.450865     0.140136    -0.785634      97.42
 O       7.103047     1.442529    -0.679316     239.95
 H       7.239885     1.850244     0.284294      27.80
 H       6.695985    -0.316113    -1.789087      28.72
 H       6.963860    -0.578628     0.086421      27.32
55
name= lig-ACN-Water-frame_265
 C      -3.835379     0.339379    -3.004727       9.93
 H      -3.994779    -0.605787    -3.595179      24.29
 C      -3.534593     1.886432    -1.116413      81.40
 H      -3.445906     2.077588     0.021821      26.32
 C      -3.574649     2.950351    -1.927683      17.12
 O      -3.285437     4.320668    -1.553908     222.35
 C      -2.785620     4.585300    -0.269832     114.63
 H      -1.963411     3.900063    -0.001770      27.57
 H      -3.739763     4.441979     0.448171      25.23
 H      -2.606835     5.607597    -0.414880      27.40
 C      -3.708205     2.732334    -3.342971       6.51
 O      -3.615456     3.717107    -4.280990      54.57
 H      -3.794974     4.632531    -3.915470      25.30
 C      -3.758488     1.395990    -3.835714      46.36
 H      -3.866591     1.237387    -4.994897      17.98
 C      -3.738888     0.533038    -1.553849     -22.40
 C      -3.849121    -0.798104    -0.754603      68.11
 H      -4.528148    -1.390493    -1.528482      21.37
 O      -4.845684    -0.665842     0.376832     152.83
 H      -4.374845    -0.438858     1.258666      28.64
 C      -2.538077    -1.510270    -0.389873      96.71
 H      -1.927480    -1.629309    -1.310705      25.89
 C      -2.711773    -2.958896     0.205897     124.79
 O      -3.555102    -3.694939    -0.666782     245.10
 H      -3.184918    -3.960455    -1.471068      32.95
 H      -3.128402    -3.156967     1.157169      26.48
 H      -1.696904    -3.340198     0.247119      27.48
 C       1.762234    -0.847854    -1.331563      40.88
 H       2.397877    -1.240535    -2.139440      18.92
 C       1.646042     1.013740     0.341814      73.73
 H       2.075043     1.917569     1.053265      19.59
 C       0.336382     0.578600     0.618625       6.60
 O      -0.537892     1.201107     1.509792     190.53
 C      -0.048106     2.518262     2.052252      94.65
 H      -1.006077     2.939297     2.537786      25.12
 H       0.750101     2.305870     2.671292      27.53
 H       0.231231     3.010936     1.053224      26.54
 C      -0.339111    -0.432033    -0.156501       7.76
 O      -1.617072    -0.695927     0.399313     183.74
 C       0.405910    -1.175587    -1.118590      71.75
 H      -0.070478    -1.990858    -1.620830      21.70
 C       2.372346     0.325138    -0.645285      32.62
 C       3.815632     0.696549    -1.125910      95.54
 H       3.836131     0.406852    -2.204983      25.02
 O       4.193168     2.048938    -1.078304     241.77
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 H       4.134128     2.348583    -0.146419      29.53
 C       4.866168    -0.069281    -0.240974      78.47
 H       4.822572     0.294985     0.858788      26.81
 O       4.688229    -1.506953    -0.189556     249.39
 H       4.903044    -1.934624    -1.140437      29.74
 C       6.510417     0.161757    -0.655325      91.06
 O       7.122115     1.456949    -0.693523     192.28
 H       7.267072     1.589119     0.291307      29.32
 H       6.584826    -0.174301    -1.695243      31.96
 H       7.247703    -0.584895     0.029692      29.89
55
name= lig-ACN-Water-frame_266
 C      -3.780897     0.328567    -2.958348      38.31
 H      -4.050631    -0.766666    -3.223952      20.91
 C      -3.546088     1.840478    -1.012667      39.42
 H      -3.326673     2.051519     0.094818      22.42
 C      -3.534129     2.985417    -1.947499       5.15
 O      -3.298152     4.257613    -1.596560     180.63
 C      -2.719206     4.674778    -0.224177      99.98
 H      -1.771606     4.048916     0.064182      24.69
 H      -3.469452     4.586251     0.710681      24.61
 H      -2.391171     5.570172    -0.170723      28.82
 C      -3.691036     2.749589    -3.343172      23.10
 O      -3.608995     3.780708    -4.276556      89.48
 H      -3.687655     4.617776    -3.885950      23.33
 C      -3.863992     1.487477    -3.838912      50.89
 H      -4.161369     1.410720    -5.003960      22.94
 C      -3.703682     0.500072    -1.577173      -8.28
 C      -3.899670    -0.808154    -0.739321      72.64
 H      -4.304962    -1.755881    -1.377840      25.25
 O      -4.814771    -0.650152     0.382865     199.80
 H      -4.260688    -0.486631     1.181317      25.48
 C      -2.575090    -1.529213    -0.480659      88.81
 H      -2.229452    -1.632605    -1.458698      27.38
 C      -2.666920    -2.931632     0.148396     119.33
 O      -3.582860    -3.804807    -0.686120     202.07
 H      -2.944573    -4.020497    -1.444162      29.34
 H      -3.018445    -2.780161     1.134028      27.35
 H      -1.673419    -3.401914     0.165823      26.91
 C       1.756686    -0.779779    -1.347246      44.95
 H       2.135121    -1.376237    -2.186837      19.70
 C       1.606771     1.027730     0.304787      79.21
 H       2.183014     1.885892     0.830368      19.84
 C       0.307927     0.583946     0.719357       4.81
 O      -0.552298     1.244761     1.570863     215.44
 C      -0.119381     2.507780     2.061994     124.16
 H      -0.892436     2.980360     2.562929      27.22
 H       0.630641     2.537451     2.798794      27.62
 H       0.191041     3.372162     1.288102      25.43
 C      -0.299783    -0.522330    -0.008655      -2.71
 O      -1.686850    -0.674862     0.376103     142.46
 C       0.400156    -1.157199    -1.073706      55.22
 H       0.007238    -1.722532    -1.834001      20.05
 C       2.352977     0.291833    -0.729337      41.12
 C       3.785570     0.606401    -1.153287      94.41
 H       3.988346     0.297299    -2.141533      27.57
 O       4.185229     2.054489    -1.068190     239.71
 H       4.461740     2.271128    -0.166910      28.49
 C       4.894673    -0.111396    -0.172606      81.04
 H       4.489018     0.175488     0.849982      25.00
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 O       4.767955    -1.553217    -0.222720     288.76
 H       4.664077    -1.811508    -1.212889      25.53
 C       6.417609     0.093959    -0.614095      90.11
 O       7.147806     1.452688    -0.632903     167.72
 H       7.325837     1.777874     0.241709      31.16
 H       6.470412    -0.266805    -1.622673      32.46
 H       7.058267    -0.713982     0.095455      28.87
55
name= lig-ACN-Water-frame_267
 C      -3.831678     0.385197    -2.948789      55.22
 H      -3.837681    -0.659866    -3.487914      22.14
 C      -3.558774     1.762705    -1.016426      92.90
 H      -3.443901     1.815303     0.073276      27.25
 C      -3.448943     2.868692    -1.872720     -23.50
 O      -3.264908     4.337487    -1.518749     169.95
 C      -2.699816     4.639291    -0.277233     107.80
 H      -1.693999     3.986907    -0.119606      24.79
 H      -3.523425     4.424850     0.560766      24.63
 H      -2.651294     5.619529    -0.416040      28.72
 C      -3.671013     2.808271    -3.338037      -1.43
 O      -3.606396     3.867190    -4.257762      83.66
 H      -3.499845     4.748403    -3.821978      20.02
 C      -3.966483     1.453567    -3.817853      43.32
 H      -4.126611     1.271266    -4.984390      22.78
 C      -3.694588     0.496419    -1.548456      28.45
 C      -3.952111    -0.791090    -0.731042      82.45
 H      -4.692111    -1.359152    -1.479313      24.37
 O      -4.750916    -0.631834     0.427181     213.44
 H      -4.254193    -0.402171     1.226176      26.33
 C      -2.530473    -1.499813    -0.565518      92.95
 H      -2.063901    -1.467827    -1.485381      28.81
 C      -2.656445    -2.930876     0.078525     111.69
 O      -3.529029    -3.876883    -0.667155     174.86
 H      -3.139627    -4.150779    -1.582247      28.23
 H      -3.198454    -2.861599     1.019501      26.65
 H      -1.622025    -3.395763     0.237946      26.07
 C       1.652773    -0.749739    -1.412039      30.11
 H       2.298444    -1.225479    -2.194301      19.58
 C       1.617904     0.966043     0.248059      68.76
 H       2.007786     1.881866     0.644767      21.12
 C       0.302097     0.586707     0.694230     -14.79
 O      -0.538669     1.270253     1.640921     190.35
 C      -0.174195     2.605214     2.141817     104.06
 H      -1.024300     2.908054     2.556777      26.98
 H       0.686404     2.421070     2.751311      26.04
 H       0.155879     3.117529     1.089680      24.43
 C      -0.340831    -0.543666     0.135709      -1.06
 O      -1.703993    -0.698394     0.310106     158.09
 C       0.336944    -1.108753    -1.008849      83.10
 H      -0.234098    -1.875021    -1.419857      23.60
 C       2.351720     0.315860    -0.749303      27.04
 C       3.905608     0.598021    -1.035033      92.51
 H       4.016571     0.304163    -2.004173      25.12
 O       4.107192     2.049285    -1.076998     248.70
 H       4.648884     2.370056    -0.283308      24.64
 C       4.884906    -0.153622    -0.188661     102.45
 H       4.921575     0.139183     0.884864      25.15
 O       4.804936    -1.594133    -0.218754     279.28
 H       4.792167    -1.904987    -1.189061      26.15
 C       6.340734     0.121337    -0.582726      97.93
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 O       7.119238     1.358230    -0.551666     210.55
 H       7.028217     1.673644     0.365392      33.10
 H       6.510581    -0.270764    -1.563876      31.92
 H       6.953670    -0.604742     0.214259      29.16
55
name= lig-ACN-Water-frame_268
 C      -3.918356     0.390091    -3.000215      39.69
 H      -3.920147    -0.659433    -3.485228      27.81
 C      -3.522626     1.797764    -1.008105      51.26
 H      -3.583541     1.983934     0.021537      25.15
 C      -3.402355     2.970514    -1.914082     -22.14
 O      -3.280717     4.235533    -1.543985     176.81
 C      -2.714709     4.605819    -0.285024     117.49
 H      -1.552617     4.271843    -0.110869      27.47
 H      -3.289012     4.184629     0.652898      26.71
 H      -2.630185     5.607982    -0.078493      30.11
 C      -3.684013     2.797439    -3.282256      22.38
 O      -3.580728     3.856259    -4.164324      -5.31
 H      -3.916247     4.817777    -3.831600      17.18
 C      -3.953767     1.544179    -3.793976      66.54
 H      -4.093754     1.376969    -4.898153      22.84
 C      -3.767115     0.481082    -1.574871     -45.24
 C      -3.894681    -0.765577    -0.767925      58.98
 H      -4.492141    -1.619591    -1.342782      23.34
 O      -4.700469    -0.607478     0.524265     166.38
 H      -4.017404    -0.454579     1.263720      27.14
 C      -2.547826    -1.529539    -0.634116      78.13
 H      -2.086676    -1.597866    -1.613906      28.91
 C      -2.684029    -2.953242    -0.001195     117.76
 O      -3.451134    -3.924785    -0.662318     244.03
 H      -3.155763    -4.000809    -1.541103      32.15
 H      -3.117847    -2.789856     1.023670      26.27
 H      -1.590622    -3.290429     0.216449      26.08
 C       1.595111    -0.719351    -1.429747      48.72
 H       1.845967    -1.390157    -2.314180      23.44
 C       1.580493     1.005691     0.303173      61.44
 H       2.003567     1.784502     0.755381      25.67
 C       0.275473     0.643815     0.715822      19.44
 O      -0.500541     1.234947     1.676057     197.41
 C      -0.151922     2.627586     2.139868     108.66
 H      -0.950279     3.094565     2.615217      27.71
 H       0.598881     2.778716     2.932424      26.59
 H       0.056118     3.456559     1.289397      27.24
 C      -0.368972    -0.476371     0.034895      12.55
 O      -1.734486    -0.710032     0.340117     134.21
 C       0.279295    -1.134042    -0.957703      67.65
 H       0.029730    -2.077083    -1.448526      24.04
 C       2.355394     0.264997    -0.734258       9.36
 C       3.822910     0.634450    -1.009143     110.69
 H       4.069123     0.296169    -1.914118      25.58
 O       4.048069     2.054583    -1.095054     259.16
 H       4.206848     2.471332    -0.135166      23.64
 C       4.942354    -0.139050    -0.100757      98.92
 H       4.674050     0.073602     0.932982      27.10
 O       4.770056    -1.597874    -0.165942     271.64
 H       4.902645    -1.941982    -1.077552      27.13
 C       6.448042     0.048386    -0.579366     100.49
 O       7.021528     1.338474    -0.455742     203.03
 H       6.964240     1.753369     0.503017      27.18
 H       6.572810    -0.244957    -1.625192      29.78
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 H       7.029269    -0.799002     0.095792      28.71
55
name= lig-ACN-Water-frame_269
 C      -3.988334     0.390990    -3.000307      35.59
 H      -4.306219    -0.605072    -3.386471      22.90
 C      -3.522253     1.830632    -1.068243      94.43
 H      -3.344431     1.915564    -0.054382      25.48
 C      -3.452721     2.906443    -1.893443      10.05
 O      -3.278370     4.268300    -1.537002     185.80
 C      -2.685972     4.548050    -0.194360     108.74
 H      -1.529892     4.279545    -0.393250      24.07
 H      -3.160420     3.909367     0.598234      25.43
 H      -3.030280     5.584355    -0.189980      26.24
 C      -3.705321     2.816143    -3.252223      19.70
 O      -3.569815     3.839109    -4.119776      -6.48
 H      -3.896231     4.816189    -3.737983      17.56
 C      -3.904151     1.559436    -3.845689      47.67
 H      -4.109150     1.673577    -4.864796      23.48
 C      -3.844134     0.578328    -1.630771       6.48
 C      -3.908823    -0.806182    -0.711813      69.62
 H      -4.616928    -1.520996    -1.338623      24.07
 O      -4.578540    -0.588916     0.540344     216.78
 H      -3.969084    -0.620365     1.394230      22.57
 C      -2.574982    -1.525706    -0.587270      78.52
 H      -2.057659    -1.450536    -1.598827      24.48
 C      -2.621819    -2.914781     0.041515     105.72
 O      -3.416180    -3.969508    -0.720909     232.42
 H      -2.998610    -4.017397    -1.627385      30.05
 H      -3.116031    -2.868049     1.084723      24.12
 H      -1.543817    -3.398348     0.033694      22.96
 C       1.583109    -0.745243    -1.378096      55.25
 H       2.254104    -1.153349    -2.205806      20.44
 C       1.611306     1.004258     0.344972      63.77
 H       2.077510     1.633183     0.909015      22.61
 C       0.235003     0.658942     0.668728       0.37
 O      -0.447327     1.292409     1.752341     206.43
 C      -0.156904     2.645749     2.143272      84.81
 H      -1.121180     2.829218     2.618210      23.76
 H       0.771662     2.531869     2.800247      23.37
 H       0.115716     3.189808     1.150403      25.38
 C      -0.466420    -0.353659    -0.060248      -2.08
 O      -1.728857    -0.737928     0.359806     167.78
 C       0.332824    -1.197353    -1.002836      63.74
 H      -0.321902    -1.963712    -1.538558      20.04
 C       2.242548     0.274017    -0.651051      24.62
 C       3.769318     0.581117    -1.064098      79.16
 H       3.862437     0.311297    -1.983174      25.25
 O       3.982371     2.112252    -1.086696     217.95
 H       4.046056     2.429376    -0.114842      23.27
 C       4.962313    -0.160498    -0.057799      89.85
 H       4.951998     0.218977     0.936448      25.04
 O       4.671764    -1.556735    -0.075529     309.87
 H       4.657202    -1.751372    -1.018724      26.86
 C       6.480876    -0.028320    -0.518676      94.78
 O       6.958515     1.407670    -0.368638     195.87
 H       6.874587     1.545535     0.689884      28.18
 H       6.437194    -0.196745    -1.619927      30.90
 H       7.260488    -0.794715    -0.041347      29.53
55
name= lig-ACN-Water-frame_270
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 C      -4.084309     0.459173    -3.041870      43.32
 H      -4.367625    -0.466767    -3.516653      24.58
 C      -3.531858     1.770699    -1.024884      51.94
 H      -3.145365     1.726608    -0.019618      23.05
 C      -3.531878     2.983452    -1.860239      16.17
 O      -3.268819     4.298479    -1.459880     246.36
 C      -2.701254     4.493661    -0.226319     135.30
 H      -1.523892     4.593236    -0.100069      25.13
 H      -3.016993     3.812194     0.560296      25.46
 H      -2.887963     5.471670     0.289532      26.90
 C      -3.691014     2.790128    -3.311628      18.82
 O      -3.577957     3.881558    -4.154080      90.43
 H      -3.453706     4.780767    -3.730393      20.11
 C      -3.906112     1.497941    -3.896089      37.28
 H      -4.008537     1.277603    -4.860124      28.18
 C      -3.868682     0.481203    -1.577951      -4.21
 C      -3.979220    -0.727883    -0.718735      85.79
 H      -4.693062    -1.460383    -1.273572      23.55
 O      -4.511245    -0.562282     0.568685     251.21
 H      -3.766602    -0.514495     1.289316      21.30
 C      -2.571303    -1.484796    -0.528476      70.77
 H      -2.143948    -1.639316    -1.613385      22.93
 C      -2.574540    -3.016198     0.022674      96.12
 O      -3.368441    -3.916007    -0.760522     243.69
 H      -2.957013    -4.143049    -1.688301      27.42
 H      -3.052310    -3.081146     1.097444      23.75
 H      -1.408824    -3.214616     0.254942      22.96
 C       1.667780    -0.785852    -1.309595      72.32
 H       2.199062    -1.402150    -2.102703      19.37
 C       1.542878     0.965524     0.438963      51.17
 H       2.068803     1.628294     1.005079      19.37
 C       0.211198     0.729020     0.653133       9.01
 O      -0.434558     1.228193     1.746162     211.71
 C      -0.112518     2.609600     2.123459     100.79
 H      -0.904518     3.221394     2.751900      22.83
 H       0.737698     2.800775     2.874445      24.43
 H       0.014711     3.323618     1.258119      26.03
 C      -0.425818    -0.355150    -0.123907       3.94
 O      -1.702741    -0.732361     0.355698     179.84
 C       0.249518    -1.107846    -1.036416      74.50
 H      -0.147509    -1.995707    -1.665455      18.76
 C       2.309418     0.303322    -0.630954      28.62
 C       3.774700     0.643951    -0.996440     103.48
 H       3.933544     0.303066    -1.867344      30.12
 O       3.886357     2.080685    -1.098232     235.25
 H       4.355941     2.408057    -0.335791      27.28
 C       4.933420    -0.133043    -0.107483      83.13
 H       4.788463     0.220378     0.862059      27.91
 O       4.524011    -1.529707     0.010823     284.96
 H       4.761661    -2.083097    -0.795539      29.42
 C       6.411445     0.087490    -0.540435     109.47
 O       6.896415     1.409842    -0.277894     202.24
 H       7.012727     1.668188     0.702277      27.14
 H       6.751039    -0.170110    -1.604216      28.43
 H       6.998625    -0.639963     0.139164      29.84
55
name= lig-ACN-Water-frame_271
 C      -4.140270     0.377017    -2.961768      59.02
 H      -4.251185    -0.602603    -3.359119      25.24
 C      -3.533545     1.769425    -1.051541      61.91
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 H      -3.383873     1.923551     0.059315      18.74
 C      -3.576103     2.905291    -1.882341      10.23
 O      -3.302316     4.292120    -1.455925     171.63
 C      -2.651230     4.476858    -0.074775     114.77
 H      -1.579165     4.408582    -0.403805      25.74
 H      -2.891990     3.666637     0.506871      26.17
 H      -3.187051     5.478847     0.187522      25.57
 C      -3.658272     2.824547    -3.330761      13.51
 O      -3.563877     3.874830    -4.225030     135.34
 H      -3.634364     4.687415    -3.787516      25.32
 C      -3.913476     1.547643    -3.882784      52.21
 H      -3.910949     1.531295    -4.908077      23.77
 C      -3.886148     0.532887    -1.629807      16.75
 C      -3.925915    -0.808729    -0.696024      78.09
 H      -4.561723    -1.605070    -1.184275      25.55
 O      -4.564729    -0.491564     0.632404     201.68
 H      -3.916733    -0.309276     1.366848      23.24
 C      -2.596659    -1.566646    -0.554991      74.47
 H      -2.043781    -1.494465    -1.597674      24.75
 C      -2.566789    -2.991118     0.028934     108.20
 O      -3.325497    -3.868485    -0.808256     264.74
 H      -2.844859    -3.993823    -1.598138      31.96
 H      -3.072735    -3.015823     1.093929      24.18
 H      -1.493379    -3.509192    -0.051456      22.81
 C       1.686438    -0.788106    -1.231327      55.66
 H       2.183045    -1.464157    -1.945737      23.21
 C       1.639323     0.949047     0.400640      57.31
 H       2.007463     1.766711     1.053998      19.50
 C       0.200824     0.669484     0.637378      -4.58
 O      -0.488858     1.213740     1.757411     191.69
 C      -0.072193     2.637180     2.130676      80.41
 H      -1.076166     2.741727     2.772595      21.66
 H       0.961547     2.513724     2.642662      23.49
 H       0.039246     3.149056     1.207710      27.93
 C      -0.418778    -0.349108    -0.056658       5.21
 O      -1.687571    -0.690656     0.314673     124.02
 C       0.340717    -0.981605    -1.132948      73.14
 H      -0.139085    -1.897733    -1.571267      21.52
 C       2.338906     0.241644    -0.570340      37.63
 C       3.782560     0.636414    -0.967351     112.36
 H       3.893263     0.313357    -1.853263      30.01
 O       3.851334     2.067187    -1.141320     243.06
 H       3.990176     2.533756    -0.283405      26.70
 C       4.781141    -0.037947    -0.128098      96.98
 H       4.797202     0.301611     0.845528      29.49
 O       4.422242    -1.508870     0.062049     245.25
 H       4.833409    -1.927766    -0.796411      27.60
 C       6.328091     0.148652    -0.496400      98.94
 O       6.864283     1.489854    -0.211085     239.11
 H       6.925814     1.572743     0.729595      30.39
 H       6.519058    -0.072279    -1.608500      28.47
 H       6.834940    -0.614941     0.147047      29.84
55
name= lig-ACN-Water-frame_272
 C      -4.055855     0.393396    -3.036306      47.78
 H      -4.277260    -0.562368    -3.476051      29.21
 C      -3.607166     1.822724    -1.110483      53.38
 H      -3.597819     1.896910     0.059236      25.77
 C      -3.498298     2.969975    -1.920608      24.89
 O      -3.359721     4.199995    -1.412637     214.90
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 C      -2.665016     4.403456    -0.105566     127.79
 H      -1.613077     4.641948    -0.089797      27.72
 H      -2.813484     3.804229     0.712771      28.00
 H      -2.995233     5.504684     0.314263      25.86
 C      -3.685702     2.807660    -3.299784      29.94
 O      -3.530730     3.844971    -4.262723      47.78
 H      -3.858979     4.763589    -4.052029      20.76
 C      -3.947724     1.503913    -3.791765      57.52
 H      -4.117307     1.428068    -4.868497      25.35
 C      -3.868413     0.477366    -1.552614     -73.54
 C      -3.930803    -0.827918    -0.600539      83.48
 H      -4.649534    -1.424549    -1.116947      24.48
 O      -4.644129    -0.448295     0.608679     197.95
 H      -4.009235    -0.510040     1.342113      27.10
 C      -2.496237    -1.528348    -0.575897      85.48
 H      -2.231498    -1.685484    -1.705281      25.56
 C      -2.544281    -2.949661     0.003535     102.75
 O      -3.353573    -3.852496    -0.866008     232.69
 H      -2.878520    -3.967485    -1.731998      29.01
 H      -2.994460    -2.962898     1.080909      24.93
 H      -1.382230    -3.178372     0.255908      24.11
 C       1.733928    -0.799670    -1.279967      38.99
 H       2.390950    -1.282496    -1.977737      21.61
 C       1.585791     0.986984     0.411113      81.56
 H       2.302067     1.834326     0.852378      19.02
 C       0.326880     0.636502     0.746514      16.47
 O      -0.505768     1.231294     1.698385     229.54
 C      -0.084017     2.503183     2.122924     113.01
 H      -0.692847     3.135655     2.963313      23.95
 H       0.905724     2.537581     2.715471      25.13
 H      -0.105292     3.231741     1.385395      29.18
 C      -0.387345    -0.369631    -0.089223       8.98
 O      -1.724657    -0.670161     0.261866     167.17
 C       0.307781    -0.987272    -1.094917      70.05
 H      -0.156454    -1.640864    -1.804563      24.77
 C       2.378099     0.203305    -0.506634      23.22
 C       3.681342     0.611965    -1.066256      92.95
 H       3.831230     0.264189    -1.940668      27.01
 O       3.853785     2.100730    -1.170998     212.17
 H       3.826594     2.445340    -0.198737      25.19
 C       4.769221     0.002435     0.044532     102.56
 H       4.482759     0.433475     0.944393      28.75
 O       4.415201    -1.411680     0.042311     280.36
 H       4.509538    -1.800600    -0.880137      27.35
 C       6.205710     0.177251    -0.426095     106.89
 O       6.819807     1.554716    -0.171361     245.35
 H       6.927825     1.788129     0.785072      29.59
 H       6.256353     0.125876    -1.558612      29.65
 H       6.889850    -0.558939    -0.064789      30.48
55
name= lig-ACN-Water-frame_273
 C      -3.934908     0.320703    -2.928795      52.59
 H      -4.209168    -0.596784    -3.463033      24.29
 C      -3.714194     1.753368    -1.088650      60.23
 H      -3.562307     1.990625     0.038938      23.37
 C      -3.446051     2.910722    -1.912122       1.61
 O      -3.375690     4.216317    -1.294432     238.97
 C      -2.682470     4.412887    -0.131792     123.41
 H      -1.689895     4.312574    -0.413809      27.15
 H      -2.976427     3.640446     0.499592      26.65
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 H      -3.149542     5.512343     0.238289      24.04
 C      -3.704126     2.840331    -3.345351      24.38
 O      -3.509694     3.788885    -4.293580      86.91
 H      -3.732493     4.765339    -3.880913      18.11
 C      -3.983577     1.528605    -3.809537      39.09
 H      -4.239079     1.293613    -4.932478      22.16
 C      -3.830929     0.457365    -1.583746      37.77
 C      -4.007550    -0.726469    -0.674572      95.42
 H      -4.469139    -1.542054    -1.110837      26.73
 O      -4.659212    -0.453254     0.610964     200.68
 H      -4.046052    -0.432166     1.396928      24.28
 C      -2.573555    -1.453145    -0.569898      72.57
 H      -2.134856    -1.375745    -1.612081      23.81
 C      -2.536247    -2.934216    -0.022603     114.48
 O      -3.333413    -3.802373    -0.859309     256.04
 H      -2.950875    -3.955160    -1.815284      28.96
 H      -3.198409    -2.948253     0.905197      23.94
 H      -1.522657    -3.519770     0.078248      23.46
 C       1.676338    -0.789651    -1.317626      47.46
 H       1.999595    -1.227093    -2.216312      21.68
 C       1.659688     0.996761     0.432833      76.92
 H       1.939327     2.026177     1.052167      17.53
 C       0.295576     0.552028     0.800314       5.89
 O      -0.538106     1.225294     1.646318     208.44
 C      -0.046301     2.525286     2.190297      92.79
 H      -0.901528     2.571536     2.974062      22.51
 H       1.026682     2.369527     2.500140      25.03
 H       0.023762     3.167083     1.393480      29.18
 C      -0.325866    -0.383810    -0.054399       7.67
 O      -1.665001    -0.597599     0.199572     183.43
 C       0.347387    -1.099622    -1.116748      58.42
 H      -0.193964    -1.606422    -1.823405      21.26
 C       2.280424     0.237445    -0.594052      33.45
 C       3.740030     0.687889    -0.979265     107.88
 H       3.969450     0.274660    -1.848911      30.38
 O       3.820383     2.096685    -1.191091     210.90
 H       4.348130     2.541606    -0.415940      25.38
 C       4.674903     0.058944     0.067102     109.19
 H       4.539091     0.299429     1.092750      29.76
 O       4.458754    -1.349530     0.048920     295.65
 H       4.628300    -1.579941    -0.881015      30.36
 C       6.180407     0.318421    -0.359030     106.36
 O       6.752887     1.577373    -0.142282     182.65
 H       6.934234     1.626703     0.899952      26.01
 H       6.080187     0.231427    -1.454068      32.66
 H       6.743277    -0.482870    -0.012298      33.12
55
name= lig-ACN-Water-frame_274
 C      -3.910172     0.344653    -3.022641      58.25
 H      -3.902281    -0.729246    -3.294912      26.67
 C      -3.699249     1.788256    -1.023775      62.65
 H      -3.756768     1.787540     0.087846      21.88
 C      -3.543999     2.880651    -1.875226      16.21
 O      -3.477403     4.209629    -1.387149     202.15
 C      -2.649305     4.372797    -0.074649     110.66
 H      -1.643115     4.365764    -0.146383      28.42
 H      -2.849924     3.787531     0.798681      26.83
 H      -2.736193     5.551260     0.336460      24.60
 C      -3.663892     2.739537    -3.303076      25.18
 O      -3.510231     3.796519    -4.300650      93.83
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 H      -3.523778     4.762095    -3.915951      21.65
 C      -3.960462     1.438271    -3.793935      76.35
 H      -4.011609     1.470104    -5.000558      18.06
 C      -3.868326     0.507325    -1.567848       5.08
 C      -3.976735    -0.763596    -0.688448      99.50
 H      -4.682754    -1.294756    -1.164124      28.07
 O      -4.626630    -0.437095     0.594390     170.56
 H      -3.870668    -0.328168     1.277084      24.58
 C      -2.570849    -1.380406    -0.584716      81.72
 H      -2.296277    -1.498063    -1.648820      26.39
 C      -2.606021    -2.887659    -0.049741     113.17
 O      -3.363148    -3.772598    -0.881731     288.39
 H      -2.883095    -3.797778    -1.685655      32.83
 H      -2.884529    -2.944125     1.023961      26.12
 H      -1.475764    -3.058020     0.010422      25.41
 C       1.649904    -0.721348    -1.417032      47.44
 H       2.300594    -1.093598    -2.169603      14.92
 C       1.584771     0.877271     0.444587      60.73
 H       2.289940     1.751538     0.853764      16.66
 C       0.328420     0.539064     0.705702      18.44
 O      -0.564524     1.218508     1.638550     195.00
 C      -0.030825     2.469990     2.237504     114.03
 H      -0.628953     2.871245     3.074500      24.51
 H       0.905894     2.336275     2.811328      24.87
 H      -0.113977     3.298857     1.623844      27.89
 C      -0.321233    -0.522333    -0.047536      12.26
 O      -1.673035    -0.500230     0.207644     153.72
 C       0.302373    -1.161426    -1.080787      83.99
 H      -0.146440    -1.976982    -1.531781      22.90
 C       2.264350     0.380592    -0.698209      31.31
 C       3.677781     0.707451    -0.898255      96.78
 H       3.987432     0.236641    -1.741216      26.04
 O       3.822687     2.161944    -1.207157     213.51
 H       4.277746     2.614795    -0.470307      26.41
 C       4.699039     0.140155     0.111709      76.91
 H       4.492549     0.550418     1.112923      27.44
 O       4.522465    -1.349929     0.048673     291.94
 H       4.806772    -1.695972    -0.819645      29.67
 C       6.121523     0.340756    -0.363285     118.52
 O       6.715819     1.662329    -0.069870     212.52
 H       6.854309     1.878425     0.986832      26.23
 H       6.336577     0.149246    -1.395351      33.24
 H       6.663150    -0.331968     0.160989      33.29
55
name= lig-ACN-Water-frame_275
 C      -3.929934     0.306146    -2.981747      46.35
 H      -3.938394    -0.636560    -3.536556      23.36
 C      -3.703965     1.800502    -0.987291      36.75
 H      -3.768795     2.015386     0.033687      16.68
 C      -3.680570     2.947615    -1.850516      18.21
 O      -3.488829     4.217897    -1.368022     203.70
 C      -2.620661     4.381651    -0.090440     104.03
 H      -1.756111     4.066876    -0.404455      29.08
 H      -3.150912     3.733925     0.653599      24.28
 H      -2.915388     5.544463    -0.003421      24.09
 C      -3.634150     2.728082    -3.293587      24.80
 O      -3.508389     3.727878    -4.199432     183.76
 H      -3.757301     4.536659    -3.831181      28.04
 C      -3.828619     1.451943    -3.880756      50.34
 H      -3.855810     1.209437    -5.044769      20.64
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 C      -3.906743     0.514726    -1.593919      46.04
 C      -3.971370    -0.697549    -0.699826     117.59
 H      -4.431857    -1.510623    -1.078938      31.67
 O      -4.513735    -0.396357     0.580114     205.77
 H      -3.886979    -0.355436     1.355045      23.81
 C      -2.598372    -1.405434    -0.613994      94.51
 H      -2.093951    -1.414200    -1.546846      30.72
 C      -2.555401    -2.773317    -0.015135     121.25
 O      -3.398040    -3.725158    -0.895337     201.27
 H      -2.983905    -3.899304    -1.768648      31.41
 H      -3.057635    -2.893295     0.921004      28.56
 H      -1.593283    -3.258043    -0.092660      26.99
 C       1.608711    -0.645658    -1.504824      60.82
 H       2.156052    -1.260101    -2.211511      26.63
 C       1.602297     0.873375     0.407856      62.02
 H       2.034374     1.497029     1.220362      22.55
 C       0.210796     0.572026     0.695567       3.20
 O      -0.528021     1.214906     1.637709     192.90
 C      -0.041240     2.411911     2.321479     115.54
 H      -0.766174     2.552778     2.993902      26.07
 H       0.954481     2.235711     2.660600      26.50
 H       0.219674     3.080388     1.521008      26.88
 C      -0.387404    -0.512461    -0.010529     -23.91
 O      -1.800133    -0.509673     0.201245     109.80
 C       0.410243    -1.223357    -1.085197      65.20
 H       0.090609    -2.153105    -1.572330      24.63
 C       2.204546     0.350307    -0.737688      23.20
 C       3.661050     0.763707    -1.010500      84.96
 H       3.884531     0.404693    -1.997051      26.38
 O       3.837976     2.234967    -1.193666     200.20
 H       3.891077     2.609211    -0.312133      27.69
 C       4.701764     0.120521     0.093317      90.20
 H       4.560732     0.357429     1.192059      25.94
 O       4.576298    -1.316951     0.117356     285.86
 H       4.699058    -1.513610    -0.854414      26.99
 C       6.218115     0.385638    -0.254497     108.93
 O       6.667573     1.730659    -0.046183     255.60
 H       6.686482     1.952288     0.968110      25.55
 H       6.250218     0.232864    -1.287506      29.85
 H       6.762455    -0.321788     0.222597      32.35
55
name= lig-ACN-Water-frame_276
 C      -3.947916     0.348390    -2.989964      67.87
 H      -4.234492    -0.663884    -3.205990      26.91
 C      -3.802863     1.797087    -1.058564      77.60
 H      -3.630088     1.792881    -0.064479      25.97
 C      -3.713578     2.917145    -1.871068      12.14
 O      -3.500264     4.274054    -1.344971     268.96
 C      -2.715232     4.369329    -0.247029     131.58
 H      -1.789775     4.024718    -0.255657      31.14
 H      -3.050729     3.933139     0.776915      26.30
 H      -2.408289     5.429858     0.124186      26.19
 C      -3.689930     2.687238    -3.264747      21.94
 O      -3.493680     3.763006    -4.128881     134.85
 H      -3.849675     4.622920    -3.786653      22.81
 C      -3.672280     1.404291    -3.833181      59.54
 H      -3.708392     1.452747    -4.946941      25.15
 C      -3.928436     0.528943    -1.605024       8.51
 C      -3.957633    -0.738443    -0.730511      89.77
 H      -4.728789    -1.251404    -1.141399      27.60
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 O      -4.424280    -0.355700     0.631225     149.57
 H      -3.652788    -0.284453     1.192064      26.42
 C      -2.556505    -1.381480    -0.678209      92.97
 H      -2.255796    -1.382016    -1.669465      28.64
 C      -2.597571    -2.865487    -0.063929     128.58
 O      -3.437063    -3.649657    -0.866827     237.40
 H      -2.866885    -3.790848    -1.730281      28.77
 H      -3.029334    -2.722485     0.876187      28.01
 H      -1.632946    -3.170087     0.228904      28.17
 C       1.597409    -0.676127    -1.517515      42.56
 H       2.026812    -1.030050    -2.497123      25.68
 C       1.532370     0.900817     0.410231      63.45
 H       2.099101     1.491182     1.004800      22.52
 C       0.200479     0.555413     0.653694      18.56
 O      -0.540540     1.168629     1.665163     206.64
 C       0.026578     2.330602     2.331090     131.47
 H      -0.631201     2.700815     2.935360      29.22
 H       0.789691     2.091906     2.992455      28.70
 H       0.069203     3.237686     1.727827      27.80
 C      -0.446498    -0.450460    -0.102841      19.31
 O      -1.790199    -0.569038     0.214582     185.48
 C       0.332356    -1.185140    -0.977143      62.31
 H      -0.199649    -1.997157    -1.613143      21.42
 C       2.257446     0.359461    -0.723130      -3.63
 C       3.725457     0.815453    -1.074230      88.44
 H       4.046523     0.433516    -2.096837      27.23
 O       3.821444     2.276450    -1.127987     170.19
 H       4.104551     2.653748    -0.228905      24.81
 C       4.713283     0.117404     0.032717      96.65
 H       4.251324     0.649465     0.944944      25.88
 O       4.582929    -1.301499     0.165684     282.82
 H       4.809087    -1.799468    -0.689148      28.50
 C       6.257174     0.412838    -0.193248     118.29
 O       6.630430     1.770776    -0.035083     218.77
 H       6.888121     1.935502     0.905741      25.79
 H       6.509009     0.191631    -1.180943      32.66
 H       6.902713    -0.176921     0.337520      34.00
55
name= lig-ACN-Water-frame_277
 C      -3.969475     0.296832    -3.020358      55.79
 H      -4.043902    -0.604278    -3.593533      23.73
 C      -3.855134     1.814056    -1.012349      62.68
 H      -3.785527     1.930187     0.031409      21.55
 C      -3.696023     2.957017    -1.831802      12.98
 O      -3.603319     4.251884    -1.463790     225.53
 C      -2.634252     4.375142    -0.194116     100.52
 H      -1.907895     3.763132    -0.451035      28.65
 H      -3.371513     4.059942     0.655419      24.20
 H      -2.563595     5.438137    -0.309702      25.89
 C      -3.680224     2.775896    -3.277462       6.93
 O      -3.487080     3.837990    -4.114892     137.95
 H      -3.653943     4.778711    -3.607419      18.82
 C      -3.647684     1.428249    -3.810655      56.68
 H      -3.548645     1.264553    -4.835461      27.21
 C      -3.964612     0.487217    -1.595170      22.74
 C      -4.014296    -0.688663    -0.683741      95.11
 H      -4.630135    -1.494461    -0.962290      24.78
 O      -4.342780    -0.356364     0.656133     236.47
 H      -3.609239    -0.126548     1.295180      22.95
 C      -2.590391    -1.479579    -0.730597      77.06
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 H      -2.110125    -1.494606    -1.637047      25.15
 C      -2.656263    -2.805325    -0.035221     139.26
 O      -3.473934    -3.663989    -0.897554     252.79
 H      -3.083232    -3.862524    -1.727672      32.57
 H      -3.192606    -2.796211     0.853929      25.63
 H      -1.759227    -3.281449    -0.053197      26.60
 C       1.569420    -0.683386    -1.380354      57.75
 H       2.001424    -1.098487    -2.361491      18.84
 C       1.589520     0.921497     0.338142      72.53
 H       1.934557     1.711427     0.779962      17.40
 C       0.259240     0.606458     0.667020      22.56
 O      -0.559801     1.127110     1.689937     221.30
 C       0.030615     2.300931     2.395577     121.16
 H      -0.693095     2.574461     3.017169      25.64
 H       0.921209     2.036995     2.793573      29.70
 H       0.529301     2.899853     1.594606      26.64
 C      -0.445894    -0.351613    -0.116801      19.76
 O      -1.727754    -0.639133     0.207556     161.30
 C       0.253424    -1.104221    -1.086267      70.12
 H      -0.318747    -1.965567    -1.657187      14.58
 C       2.302690     0.334420    -0.762258      56.27
 C       3.727680     0.780218    -1.041123      84.85
 H       3.972150     0.516323    -2.188745      24.31
 O       3.822149     2.292458    -1.054559     140.62
 H       4.334294     2.571412    -0.188017      22.97
 C       4.740210     0.188236    -0.035391     100.99
 H       4.606793     0.555444     1.061606      25.20
 O       4.552595    -1.300393     0.213772     270.98
 H       4.873951    -1.628556    -0.706862      26.92
 C       6.244241     0.369303    -0.206663     105.93
 O       6.641669     1.836618    -0.019100     187.54
 H       6.777595     2.060272     0.939718      29.60
 H       6.629136    -0.018982    -1.087050      33.50
 H       6.523158    -0.137274     0.658260      33.45
55
name= lig-ACN-Water-frame_278
 C      -3.913072     0.342551    -3.002524      56.70
 H      -3.775615    -0.681459    -3.351358      23.76
 C      -3.879612     1.799214    -1.014070      43.92
 H      -4.121342     1.966416     0.070195      18.36
 C      -3.737244     2.897681    -1.907689       1.07
 O      -3.632910     4.264045    -1.449321     281.49
 C      -2.715904     4.425291    -0.305208     104.65
 H      -1.887050     3.773311    -0.242866      27.59
 H      -3.152526     4.235500     0.772524      22.37
 H      -2.235162     5.317283    -0.163919      26.21
 C      -3.603521     2.788615    -3.293313      19.92
 O      -3.476565     3.907223    -4.130691     210.51
 H      -3.581791     4.766716    -3.607499      25.45
 C      -3.736032     1.522410    -3.837116      60.91
 H      -3.557041     1.462368    -4.817023      20.70
 C      -4.044378     0.491221    -1.613913      10.75
 C      -3.961554    -0.745166    -0.626865      92.87
 H      -4.775081    -1.383614    -0.970172      25.72
 O      -4.338312    -0.358180     0.719261     205.18
 H      -3.477601    -0.249742     1.267517      21.57
 C      -2.619825    -1.417888    -0.639256     106.65
 H      -2.371295    -1.519364    -1.670495      26.31
 C      -2.712598    -2.864473    -0.071395     115.34
 O      -3.565505    -3.733635    -0.932256     242.31
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 H      -3.048875    -3.794524    -1.757904      31.27
 H      -3.107170    -2.793862     0.911074      26.16
 H      -1.771680    -3.149572     0.164791      27.93
 C       1.633391    -0.753828    -1.408264      57.87
 H       2.223898    -1.557810    -1.981987      16.66
 C       1.632200     1.051327     0.313914      57.84
 H       2.153096     1.796814     0.792628      16.13
 C       0.263333     0.621332     0.659137       8.61
 O      -0.508021     1.131949     1.715182     224.81
 C       0.094420     2.220676     2.395455     127.76
 H      -0.582487     2.742900     3.055270      24.25
 H       0.831491     1.922722     2.971869      28.26
 H       0.174178     3.125907     1.732114      24.38
 C      -0.405530    -0.364444    -0.136169      21.04
 O      -1.730838    -0.692694     0.204631     201.82
 C       0.232598    -0.946164    -1.226890      97.33
 H      -0.121653    -1.846522    -1.853184      19.26
 C       2.246198     0.307721    -0.690586      27.31
 C       3.706609     0.790634    -1.013506      71.71
 H       4.057802     0.370329    -2.144336      21.11
 O       3.835507     2.229903    -1.018149     230.71
 H       3.904234     2.630652    -0.036885      22.30
 C       4.727034     0.162823     0.011030      86.66
 H       4.356457     0.717743     0.979093      23.69
 O       4.536526    -1.231990     0.189985     323.38
 H       4.593050    -1.705930    -0.702430      26.74
 C       6.260887     0.416707    -0.142759     113.85
 O       6.647511     1.806752    -0.035057     257.63
 H       6.947007     1.863090     0.939306      28.41
 H       6.698415     0.051761    -1.039447      32.18
 H       6.843911    -0.166353     0.595945      30.99
55
name= lig-ACN-Water-frame_279
 C      -3.828250     0.444260    -2.990397      48.25
 H      -3.861179    -0.572197    -3.465513      23.06
 C      -3.996321     1.824566    -1.103092      47.31
 H      -4.031507     1.927769     0.072634      19.38
 C      -3.757804     2.945033    -1.869906      10.21
 O      -3.631848     4.261059    -1.386944     275.33
 C      -2.740120     4.459556    -0.330402     112.42
 H      -2.012729     3.668792    -0.464243      26.77
 H      -3.409508     4.434965     0.628928      23.85
 H      -2.455383     5.375229    -0.554621      27.05
 C      -3.604093     2.826597    -3.330088      13.99
 O      -3.431159     3.902577    -4.139848     112.88
 H      -3.808641     4.693230    -3.833828      22.32
 C      -3.782045     1.504013    -3.906808      54.94
 H      -3.843432     1.395632    -4.919153      22.94
 C      -4.013991     0.513172    -1.553920      36.41
 C      -4.031481    -0.689503    -0.600868      88.75
 H      -4.696457    -1.560169    -0.959585      25.38
 O      -4.376743    -0.361496     0.781012     207.33
 H      -3.645917    -0.362018     1.463711      23.07
 C      -2.629470    -1.453894    -0.612089      79.44
 H      -2.167300    -1.336047    -1.610601      23.86
 C      -2.773303    -2.945981    -0.067970     124.80
 O      -3.533460    -3.755283    -0.937425     166.43
 H      -3.164019    -3.831557    -1.914916      28.67
 H      -3.423617    -2.975388     0.797838      25.31
 H      -1.889123    -3.444038    -0.044217      27.66
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 C       1.716644    -0.759325    -1.418851      35.99
 H       2.419391    -1.382956    -2.060802      18.14
 C       1.497878     1.075548     0.301014      79.39
 H       2.001261     1.806682     1.002661      20.23
 C       0.261581     0.637871     0.626711      17.50
 O      -0.446744     1.122322     1.714283     218.90
 C       0.119826     2.273318     2.456462     108.10
 H      -0.692032     2.298603     3.228256      22.32
 H       1.049089     2.076166     2.809538      28.34
 H       0.457843     3.049236     1.736539      25.10
 C      -0.393153    -0.373229    -0.204603       5.36
 O      -1.693887    -0.677956     0.244568     189.65
 C       0.293576    -0.915677    -1.327882      60.93
 H      -0.406931    -1.518097    -1.900742      20.80
 C       2.312592     0.311888    -0.665889      40.88
 C       3.732924     0.733226    -0.944601      78.03
 H       3.992192     0.474676    -2.191513      21.44
 O       3.811860     2.179490    -1.001022     184.48
 H       3.893387     2.551438    -0.076683      26.64
 C       4.712928     0.188523     0.121941     105.66
 H       4.397459     0.528231     1.183796      26.37
 O       4.493004    -1.237712     0.158727     313.98
 H       4.749185    -1.534527    -0.767772      28.58
 C       6.266063     0.422086    -0.124093     102.86
 O       6.680262     1.801900     0.003051     242.12
 H       7.112612     2.070977     0.893498      26.73
 H       6.310346     0.163771    -1.171056      33.56
 H       6.839678    -0.265377     0.575856      30.87
55
name= lig-ACN-Water-frame_280
 C      -3.829987     0.380405    -2.991924      51.46
 H      -3.991712    -0.619150    -3.514828      23.43
 C      -4.077465     1.906347    -1.045011      39.85
 H      -4.073569     2.142527     0.120641      20.76
 C      -3.770939     2.984664    -1.944342      12.40
 O      -3.731979     4.258426    -1.428720     247.66
 C      -2.728534     4.528227    -0.288117     101.17
 H      -1.811994     3.855888    -0.118804      26.75
 H      -3.141791     4.554695     0.759787      26.74
 H      -2.317099     5.386428    -0.403860      28.54
 C      -3.714373     2.823153    -3.330876      20.29
 O      -3.370755     3.899262    -4.187017     179.44
 H      -3.917685     4.695126    -3.998055      20.66
 C      -3.770212     1.549986    -3.861449      41.72
 H      -3.913491     1.331793    -4.915612      24.81
 C      -3.936300     0.555588    -1.598848      -6.67
 C      -4.006056    -0.666352    -0.559952      73.16
 H      -4.903330    -1.327608    -0.956765      22.54
 O      -4.467154    -0.362198     0.800250     181.01
 H      -3.657839    -0.279604     1.321671      26.28
 C      -2.609404    -1.485612    -0.569531      88.81
 H      -2.306724    -1.671930    -1.658760      22.49
 C      -2.772674    -2.956331    -0.058131     110.81
 O      -3.526793    -3.801526    -1.046926     223.09
 H      -2.996424    -3.636404    -1.858813      30.49
 H      -3.230382    -2.951634     0.956169      24.74
 H      -1.803580    -3.262383     0.258677      25.90
 C       1.722335    -0.645855    -1.416700      54.08
 H       2.144714    -0.957986    -2.379607      13.50
 C       1.544824     0.984294     0.233679      58.23
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 H       1.959988     1.968543     0.827502      17.82
 C       0.191494     0.606961     0.571579      14.05
 O      -0.411988     1.118583     1.726372     220.98
 C       0.163945     2.266827     2.488747     102.82
 H      -0.485329     2.629725     3.421401      22.80
 H       1.082761     2.031318     2.890571      26.72
 H      -0.024979     3.196094     1.952132      25.60
 C      -0.414826    -0.338393    -0.246220      23.24
 O      -1.656384    -0.680114     0.252629     183.62
 C       0.345007    -0.961329    -1.323111      85.56
 H       0.097046    -1.593029    -2.092668      22.20
 C       2.304118     0.328324    -0.648684      50.92
 C       3.763010     0.739211    -0.822716      75.70
 H       4.272909     0.059418    -1.822123      23.05
 O       3.778538     2.199876    -0.989672     130.47
 H       4.099004     2.582517    -0.175029      27.13
 C       4.731063     0.174859     0.239458      99.75
 H       4.526691     0.513279     1.283581      26.93
 O       4.480781    -1.311249     0.125873     264.54
 H       4.856891    -1.587767    -0.768855      30.78
 C       6.159879     0.415658    -0.142585     100.55
 O       6.726305     1.848104     0.076853     217.55
 H       6.954100     1.851015     1.047060      29.58
 H       6.500727     0.217764    -1.188288      32.38
 H       6.845739    -0.330809     0.454954      30.22
55
name= lig-ACN-Water-frame_281
 C      -3.889439     0.382052    -2.965308      53.52
 H      -3.784291    -0.713283    -3.264346      22.83
 C      -4.011797     1.901955    -1.089177      69.87
 H      -4.277398     2.084457     0.002997      22.35
 C      -3.865375     2.995832    -1.916772       1.54
 O      -3.732697     4.367015    -1.370748     236.36
 C      -2.756378     4.592869    -0.274307     109.23
 H      -2.022868     3.701597    -0.460481      25.47
 H      -3.371584     4.528833     0.594606      26.50
 H      -2.449333     5.545427    -0.420402      27.55
 C      -3.757804     2.860495    -3.366417       0.05
 O      -3.355989     3.879407    -4.242528      60.91
 H      -3.695134     4.846406    -3.896644      18.59
 C      -3.794346     1.461455    -3.817825      49.54
 H      -3.579796     1.518147    -4.946894      21.55
 C      -3.911032     0.609401    -1.517610      14.70
 C      -3.952097    -0.649383    -0.588103      76.25
 H      -4.733023    -1.424847    -1.115225      21.92
 O      -4.499729    -0.338593     0.757903     162.91
 H      -3.869128    -0.035228     1.460206      22.86
 C      -2.685082    -1.485448    -0.532942      83.49
 H      -2.237847    -1.368221    -1.602398      21.07
 C      -2.758949    -2.940915    -0.002929     114.69
 O      -3.436174    -3.772774    -1.085964     200.77
 H      -3.028285    -3.685766    -1.928054      30.84
 H      -3.541810    -3.081747     0.792752      22.41
 H      -1.777235    -3.426001     0.054591      23.37
 C       1.679269    -0.551760    -1.583488      51.72
 H       2.297416    -0.999316    -2.334264      25.47
 C       1.545861     1.000660     0.333191      65.38
 H       2.149527     1.978398     0.861064      15.39
 C       0.261325     0.665310     0.558934       6.52
 O      -0.425373     1.122874     1.748631     202.95
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 C       0.147388     2.260270     2.478467      97.07
 H      -0.537947     2.034714     3.436003      20.75
 H       1.228734     2.188687     2.604845      23.51
 H       0.182856     3.130348     1.867863      25.77
 C      -0.424577    -0.386209    -0.274077       7.38
 O      -1.704662    -0.759408     0.199607     201.28
 C       0.343791    -0.994109    -1.256316      58.57
 H      -0.178686    -1.726567    -1.733358      19.04
 C       2.363244     0.338904    -0.661124      33.73
 C       3.757437     0.761918    -0.730884      68.99
 H       4.134517     0.554724    -1.986862      16.87
 O       3.792481     2.228484    -0.969669     178.76
 H       3.972020     2.666856    -0.085613      24.82
 C       4.710020     0.066962     0.275287     110.99
 H       4.473481     0.279876     1.286825      25.10
 O       4.528354    -1.344843     0.144698     344.40
 H       4.618703    -1.614568    -0.834456      24.41
 C       6.235380     0.477286    -0.126076      85.38
 O       6.679962     1.811719     0.188704     258.46
 H       7.098795     1.909389     1.061661      30.38
 H       6.176075     0.279935    -1.261633      31.74
 H       6.926156    -0.275514     0.485065      28.44
55
name= lig-ACN-Water-frame_282
 C      -3.887731     0.410809    -2.868089      44.04
 H      -3.772955    -0.580576    -3.346827      24.64
 C      -3.956658     1.955197    -1.045887      24.19
 H      -4.044210     2.089913     0.027626      20.36
 C      -3.918105     3.170859    -1.905813       7.76
 O      -3.769401     4.423938    -1.395141     270.75
 C      -2.877919     4.570681    -0.310298     113.40
 H      -1.855708     3.963267    -0.270802      25.35
 H      -3.194489     4.448079     0.662347      25.85
 H      -2.475233     5.589288    -0.366492      25.92
 C      -3.726675     2.839629    -3.323883      26.47
 O      -3.394994     3.810233    -4.259634     178.75
 H      -3.580151     4.772095    -3.846810      21.97
 C      -3.793712     1.526665    -3.822124      52.94
 H      -3.549346     1.019531    -4.852210      22.59
 C      -3.936238     0.545786    -1.522264      34.76
 C      -3.992948    -0.622095    -0.569205      79.91
 H      -4.810892    -1.434161    -0.996624      23.35
 O      -4.536341    -0.307714     0.681044     221.44
 H      -3.708103    -0.151313     1.275419      23.89
 C      -2.655541    -1.462964    -0.590653      80.60
 H      -2.433119    -1.685348    -1.663897      24.50
 C      -2.831174    -2.964090    -0.088687     111.57
 O      -3.398039    -3.747767    -1.038938     266.70
 H      -2.823769    -3.555268    -1.849195      27.50
 H      -3.364275    -2.978660     0.918341      24.14
 H      -1.800389    -3.201733     0.389678      23.97
 C       1.656449    -0.512390    -1.626757      44.55
 H       2.211976    -1.132176    -2.260328      26.44
 C       1.602875     1.003203     0.368501      60.02
 H       2.131510     1.602432     1.319689      16.43
 C       0.240365     0.654677     0.614106      25.28
 O      -0.440213     1.109666     1.671174     212.02
 C       0.132831     2.200457     2.441134     114.27
 H      -0.292908     2.443511     3.551610      23.09
 H       1.204044     1.973870     2.714793      22.93
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 H      -0.197739     3.107344     2.062248      26.05
 C      -0.379856    -0.352362    -0.135366      10.83
 O      -1.668362    -0.764944     0.242505     181.11
 C       0.309193    -0.997723    -1.260489      60.21
 H      -0.108227    -1.844102    -1.789477      19.22
 C       2.251086     0.384984    -0.705006       7.84
 C       3.765783     0.800553    -0.847779      55.24
 H       4.250831     0.172305    -1.915336      20.46
 O       3.827005     2.281343    -0.851310     156.05
 H       4.085731     2.572393     0.141993      19.29
 C       4.766925     0.058917     0.246079     112.27
 H       4.512533     0.323783     1.220571      26.58
 O       4.589360    -1.402970     0.156818     300.52
 H       4.816832    -1.670050    -0.808775      25.28
 C       6.252440     0.441192    -0.045582      96.07
 O       6.609136     1.810157     0.266821     257.20
 H       7.058619     1.829250     1.180269      27.00
 H       6.490805     0.498064    -1.199013      29.72
 H       7.057542    -0.407483     0.239632      29.46
55
name= lig-ACN-Water-frame_283
 C      -3.863575     0.437046    -2.914503      48.22
 H      -4.085775    -0.545444    -3.242899      23.33
 C      -3.934646     2.005573    -0.993285      76.84
 H      -3.780753     2.225527    -0.015896      22.35
 C      -3.893230     3.026006    -1.920364      12.56
 O      -3.835357     4.468554    -1.470453     245.40
 C      -2.899763     4.602002    -0.263567     100.75
 H      -2.019812     3.920857    -0.595308      24.15
 H      -3.439941     4.285348     0.505225      26.17
 H      -2.796058     5.779514    -0.119822      23.94
 C      -3.697471     2.857237    -3.271203      22.12
 O      -3.446162     3.773245    -4.262822      85.10
 H      -3.739470     4.680232    -4.078950      21.25
 C      -3.756762     1.513637    -3.723476      54.13
 H      -3.847315     1.704925    -4.878381      21.41
 C      -3.989387     0.727722    -1.476990       6.33
 C      -4.032512    -0.661081    -0.633889      66.32
 H      -4.879152    -1.349681    -1.210610      24.30
 O      -4.535024    -0.275062     0.703487     157.30
 H      -3.854839    -0.185549     1.436026      23.78
 C      -2.638797    -1.450295    -0.604664      78.26
 H      -2.133799    -1.260886    -1.526894      24.01
 C      -2.798795    -2.823111     0.017240     106.34
 O      -3.449371    -3.798982    -0.988481     181.83
 H      -2.985065    -3.831939    -1.939811      26.66
 H      -3.621751    -2.815112     0.773693      23.87
 H      -1.789854    -3.373537     0.183974      22.82
 C       1.596350    -0.530612    -1.500938      50.15
 H       2.015523    -0.822568    -2.423430      17.35
 C       1.610555     0.912823     0.366975      69.59
 H       2.368022     1.484319     1.049595      16.61
 C       0.279456     0.584893     0.645010      17.06
 O      -0.520137     1.141447     1.700143     203.16
 C       0.079793     2.201944     2.472774     109.52
 H      -0.557827     1.973991     3.409822      22.00
 H       1.269448     2.153375     2.554337      21.47
 H       0.105063     3.085717     1.917990      25.87
 C      -0.365294    -0.432670    -0.171734      20.50
 O      -1.626483    -0.734106     0.316923     160.45
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 C       0.292056    -0.908741    -1.224649      80.10
 H      -0.193934    -1.667148    -1.949750      22.03
 C       2.284859     0.466447    -0.788882      33.63
 C       3.770766     0.755633    -0.886546      70.93
 H       4.144889     0.748782    -2.163694      22.61
 O       3.883600     2.264183    -0.745641     116.48
 H       4.455631     2.533206     0.102580      19.89
 C       4.789216     0.062945     0.133043      85.65
 H       4.509723     0.386728     1.112263      27.02
 O       4.662930    -1.420144     0.149926     277.48
 H       5.098548    -1.811904    -0.664381      29.16
 C       6.279579     0.403826    -0.084588      80.31
 O       6.593299     1.801679     0.338968     263.36
 H       6.795387     1.952213     1.347520      27.63
 H       6.473542     0.187110    -1.233908      28.62
 H       6.851998    -0.284155     0.696244      28.79
55
name= lig-ACN-Water-frame_284
 C      -3.936762     0.475615    -2.863803      62.42
 H      -4.035470    -0.476530    -3.253027      27.41
 C      -3.909421     2.020813    -0.924190      47.98
 H      -4.018171     2.097982     0.095015      22.63
 C      -3.794512     3.160301    -1.832809       8.91
 O      -3.853641     4.430863    -1.511586     267.65
 C      -3.052414     4.610070    -0.313876     113.61
 H      -1.947823     4.318938    -0.386922      26.30
 H      -3.321171     4.129965     0.506485      28.31
 H      -2.925176     5.820591    -0.031204      23.89
 C      -3.686952     2.855596    -3.275794       8.57
 O      -3.513379     3.812071    -4.266802     117.52
 H      -3.802477     4.642472    -3.971899      23.89
 C      -3.738844     1.551439    -3.798644      53.43
 H      -3.836790     1.220631    -4.878563      22.66
 C      -3.973722     0.638996    -1.491827       8.22
 C      -3.981948    -0.497893    -0.624950      62.52
 H      -4.675247    -1.408533    -1.049184      22.68
 O      -4.549628    -0.311077     0.737649     189.33
 H      -3.750059    -0.201412     1.268421      26.88
 C      -2.602392    -1.320397    -0.565654      91.00
 H      -2.323465    -1.560173    -1.536148      25.61
 C      -2.819556    -2.830755    -0.034172      97.50
 O      -3.544973    -3.805777    -0.865853     240.53
 H      -3.006712    -3.731543    -1.724238      28.86
 H      -3.339220    -2.706825     0.944628      24.09
 H      -1.791477    -3.162140     0.456923      23.21
 C       1.641668    -0.512877    -1.572212      35.96
 H       2.076939    -0.849097    -2.517585      14.70
 C       1.636662     0.889770     0.413810      89.14
 H       1.925667     1.768542     0.944127      13.45
 C       0.309667     0.519463     0.700871      20.75
 O      -0.513161     1.132445     1.663840     223.66
 C       0.043066     2.218680     2.499566     103.81
 H      -0.472403     2.464704     3.470231      23.49
 H       1.080683     1.792947     2.925502      22.58
 H      -0.131636     3.164736     2.066646      25.33
 C      -0.430528    -0.397139    -0.061278      15.12
 O      -1.693966    -0.724594     0.355544     197.23
 C       0.266435    -0.925399    -1.287744      90.95
 H      -0.350135    -1.626527    -2.056141      17.73
 C       2.357161     0.412130    -0.741554      32.70
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 C       3.804639     0.843559    -0.951325      76.95
 H       4.130610     0.409026    -2.168739      21.56
 O       3.953688     2.229188    -0.716140     212.36
 H       4.275158     2.401954     0.264354      21.69
 C       4.745544     0.011381    -0.005822      82.84
 H       4.388806     0.311142     1.005944      25.56
 O       4.742386    -1.400125     0.128324     284.85
 H       4.887636    -1.735530    -0.797267      28.59
 C       6.288440     0.425169    -0.027827      85.45
 O       6.609165     1.765983     0.295490     317.43
 H       7.008863     1.744656     1.206493      30.77
 H       6.945512     0.264672    -0.990517      28.38
 H       6.793007    -0.364433     0.684659      29.66
55
name= lig-ACN-Water-frame_285
 C      -3.992769     0.477403    -2.881309      60.13
 H      -3.932402    -0.501445    -3.224016      26.54
 C      -3.902710     1.985320    -0.989107      85.84
 H      -4.095286     2.173312     0.068147      24.12
 C      -3.738283     3.036025    -1.908299      11.30
 O      -3.828510     4.465974    -1.473099     247.47
 C      -3.122921     4.724460    -0.275375     113.21
 H      -2.064895     4.573758    -0.548626      25.95
 H      -3.498432     4.135735     0.459753      28.33
 H      -3.577584     5.888070    -0.019640      23.26
 C      -3.673938     2.856854    -3.305562      10.66
 O      -3.586838     3.899047    -4.238926     129.31
 H      -3.735565     4.835920    -3.917019      21.49
 C      -3.780008     1.510762    -3.804356      47.08
 H      -3.553614     1.357742    -4.839909      22.94
 C      -3.931751     0.759636    -1.472315       7.05
 C      -3.941281    -0.556280    -0.502737      73.07
 H      -4.739578    -1.211115    -1.141267      21.68
 O      -4.521803    -0.340154     0.751206     187.98
 H      -3.966202    -0.096842     1.536407      22.93
 C      -2.685941    -1.355721    -0.554365      97.01
 H      -2.238550    -1.146597    -1.454813      26.92
 C      -2.853298    -2.800372     0.037884     117.59
 O      -3.597799    -3.720237    -0.739851     218.16
 H      -3.252258    -3.910601    -1.574226      32.68
 H      -3.409279    -2.816208     0.986564      24.11
 H      -1.794599    -3.241075    -0.047377      23.19
 C       1.602635    -0.488869    -1.619227      56.66
 H       2.148462    -1.010762    -2.453577      25.18
 C       1.648151     0.946021     0.428475      65.90
 H       2.076472     1.707494     0.890865      21.39
 C       0.293007     0.509787     0.764799       1.19
 O      -0.479171     1.151919     1.685590     188.04
 C      -0.010319     2.221475     2.556127     102.51
 H      -0.822430     2.190735     3.198941      24.02
 H       1.146087     2.108877     2.976178      24.32
 H       0.279849     3.034974     1.919016      26.45
 C      -0.354485    -0.447724    -0.127591      15.03
 O      -1.732439    -0.689444     0.351023     171.70
 C       0.281372    -0.864492    -1.252874      69.21
 H      -0.246287    -1.653476    -1.984883      20.57
 C       2.313444     0.284703    -0.662377       8.06
 C       3.814890     0.769077    -0.991472      59.04
 H       4.169623     0.801407    -2.268223      19.14
 O       4.021852     2.239219    -0.742822     198.67
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 H       4.147153     2.413014     0.208998      26.92
 C       4.825020     0.077872     0.014578     104.64
 H       4.394839     0.410209     1.024928      23.26
 O       4.757027    -1.429062     0.000532     284.06
 H       4.907147    -1.818538    -0.918560      25.89
 C       6.318658     0.366753    -0.016147      93.60
 O       6.673257     1.783412     0.261986     262.81
 H       7.088770     1.890629     1.118541      30.38
 H       6.594116     0.018907    -1.089898      28.46
 H       6.760839    -0.256301     0.824087      29.01
55
name= lig-ACN-Water-frame_286
 C      -3.937532     0.433387    -2.871396      57.91
 H      -4.079698    -0.589155    -3.211100      26.42
 C      -3.890418     2.078539    -1.035026      45.88
 H      -3.772863     2.369491     0.083284      22.49
 C      -3.753056     3.117309    -1.934731      22.57
 O      -3.832163     4.395607    -1.533191     246.51
 C      -3.204102     4.873184    -0.189284     100.44
 H      -2.143097     5.009176    -0.134344      28.44
 H      -3.326198     4.223660     0.629530      28.52
 H      -3.576328     6.047402     0.155457      23.64
 C      -3.693923     2.881070    -3.372831       4.42
 O      -3.615782     3.896576    -4.208075      57.09
 H      -4.053187     4.803220    -3.833747      19.33
 C      -3.788504     1.549185    -3.808433      64.09
 H      -3.809980     1.450076    -4.837111      24.66
 C      -3.922934     0.613584    -1.455109     -10.67
 C      -4.046323    -0.547949    -0.554614      63.60
 H      -4.851216    -1.343743    -0.946882      21.82
 O      -4.555762    -0.347118     0.839303     184.71
 H      -3.703620    -0.176417     1.385195      24.67
 C      -2.685261    -1.385536    -0.528523      78.28
 H      -2.482775    -1.671564    -1.519599      27.05
 C      -2.768492    -2.780000     0.080833     109.52
 O      -3.748204    -3.661679    -0.677939     177.04
 H      -3.187802    -3.787266    -1.515455      29.42
 H      -3.080003    -2.636229     1.107576      26.71
 H      -1.745390    -3.211222     0.267437      26.03
 C       1.585168    -0.505856    -1.531697      43.06
 H       2.058904    -0.851208    -2.530997      21.70
 C       1.636370     0.905099     0.404849      66.53
 H       2.184004     1.403220     1.039395      25.13
 C       0.351869     0.565974     0.706415      22.23
 O      -0.471077     1.120301     1.747325     214.97
 C      -0.007897     2.242751     2.544870     115.96
 H      -0.735834     2.608321     3.161246      26.96
 H       0.712057     1.785003     3.369481      24.81
 H       0.119533     3.197787     1.998530      25.99
 C      -0.379093    -0.408493    -0.046831      11.42
 O      -1.642358    -0.643106     0.314109     142.41
 C       0.263678    -0.887536    -1.289009      70.18
 H      -0.291994    -1.646774    -1.949617      21.62
 C       2.365597     0.332185    -0.674808      27.48
 C       3.827238     0.746849    -0.876781      71.97
 H       3.975764     0.349578    -2.130867      22.07
 O       4.026624     2.238001    -0.813642     170.56
 H       4.297441     2.467681     0.083351      27.79
 C       4.833928     0.033127     0.056117     104.80
 H       4.495591     0.179880     1.171291      25.39
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 O       4.733142    -1.418703    -0.135044     262.27
 H       5.088629    -1.566258    -1.079390      28.22
 C       6.363680     0.364966    -0.028664     104.29
 O       6.767864     1.787267     0.191548     217.70
 H       6.941447     1.778441     1.175798      27.53
 H       6.884323     0.106626    -1.001698      30.66
 H       6.884305    -0.288383     0.689511      31.41
55
name= lig-ACN-Water-frame_287
 C      -3.858023     0.450801    -2.878171      49.39
 H      -4.088992    -0.518293    -3.411753      22.14
 C      -3.814817     1.953828    -1.049546      57.76
 H      -3.803795     2.096381     0.137793      20.13
 C      -3.781102     3.119360    -1.910509      10.26
 O      -3.776529     4.506615    -1.489261     259.46
 C      -3.287501     4.971068    -0.163518     107.17
 H      -2.319063     5.150064    -0.405879      26.55
 H      -3.588664     4.287874     0.682699      23.84
 H      -4.088246     5.889920    -0.154220      21.95
 C      -3.763587     2.854278    -3.279951      20.60
 O      -3.618912     3.880417    -4.275736      53.44
 H      -3.901360     4.927215    -4.026328      16.85
 C      -3.816837     1.502284    -3.787879      52.77
 H      -4.086438     1.217314    -4.738107      24.54
 C      -3.961570     0.701883    -1.494761      35.84
 C      -4.099093    -0.615254    -0.498371      75.04
 H      -4.825036    -1.337730    -1.060221      23.34
 O      -4.577902    -0.342808     0.838597     248.28
 H      -3.889144    -0.182096     1.581822      21.51
 C      -2.634755    -1.417791    -0.519649      78.57
 H      -2.229076    -1.361200    -1.518149      23.83
 C      -2.762801    -2.806610     0.214684     114.96
 O      -3.777690    -3.536475    -0.604784     187.36
 H      -3.485062    -3.850271    -1.540299      29.21
 H      -3.223572    -2.854317     1.192056      25.15
 H      -1.849498    -3.338564     0.080231      25.46
 C       1.631116    -0.520225    -1.508614      49.60
 H       2.074655    -0.841160    -2.526976      15.99
 C       1.735025     0.877209     0.489337      66.82
 H       2.135287     1.501311     1.215275      14.09
 C       0.273379     0.621111     0.696625      13.98
 O      -0.468017     1.084872     1.798720     202.09
 C      -0.036019     2.273253     2.575640     107.99
 H      -0.908077     2.585313     2.998581      24.15
 H       0.872954     2.062743     3.299810      23.17
 H       0.619314     2.849775     1.897324      23.49
 C      -0.348172    -0.339357    -0.139607      20.86
 O      -1.691422    -0.638720     0.254762     190.00
 C       0.252350    -0.892324    -1.211462      67.41
 H      -0.294147    -1.447670    -1.937475      20.43
 C       2.345965     0.411476    -0.685953      29.02
 C       3.847326     0.761290    -0.787538      71.57
 H       4.394085     0.338206    -1.901479      23.10
 O       4.001157     2.183515    -0.916913     180.55
 H       4.392394     2.555169    -0.038519      22.75
 C       4.849010    -0.061058     0.105564      67.99
 H       4.599065     0.037364     1.264066      24.67
 O       4.722490    -1.397272    -0.236915     341.51
 H       4.830763    -1.765225    -1.193644      28.14
 C       6.442253     0.400076    -0.076419     101.65
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 O       6.861963     1.743255     0.157506     251.46
 H       7.059639     2.023196     1.132169      26.53
 H       6.677256     0.147269    -1.124670      33.82
 H       6.935453    -0.236509     0.624266      32.23
55
name= lig-ACN-Water-frame_288
 C      -3.882803     0.416314    -2.896970      50.04
 H      -3.822613    -0.720430    -3.164660      23.00
 C      -3.774857     1.982082    -0.949302      45.71
 H      -3.901596     2.086913     0.223105      19.16
 C      -3.762490     3.106662    -1.809768       3.61
 O      -3.748104     4.532466    -1.502697     257.46
 C      -3.441452     5.038076    -0.221009     122.07
 H      -2.477806     5.294763     0.018844      29.27
 H      -3.534230     4.215352     0.604950      24.58
 H      -3.916749     6.037735     0.162865      24.62
 C      -3.813859     2.891976    -3.308559       5.73
 O      -3.629703     3.802936    -4.331371     112.80
 H      -3.754040     4.770243    -3.948151      20.13
 C      -3.878753     1.549690    -3.755145      54.57
 H      -3.758905     1.577285    -4.832841      23.40
 C      -3.949143     0.588787    -1.476063      11.76
 C      -3.970145    -0.610334    -0.510737      93.52
 H      -4.766019    -1.290758    -0.899774      23.86
 O      -4.621504    -0.358548     0.777884     210.56
 H      -3.925706    -0.171960     1.444945      25.02
 C      -2.657304    -1.392961    -0.445751      92.14
 H      -2.442248    -1.693040    -1.509423      24.43
 C      -2.798784    -2.837798     0.174024     127.10
 O      -3.819190    -3.454723    -0.538343     235.61
 H      -3.352483    -3.636234    -1.324137      32.84
 H      -3.086866    -2.624175     1.201108      26.69
 H      -1.884180    -3.346209     0.229048      27.35
 C       1.663175    -0.453494    -1.516607      48.96
 H       2.218701    -0.936194    -2.362110      20.81
 C       1.634077     0.897923     0.589964      49.09
 H       2.358265     1.530535     1.146416      16.51
 C       0.311750     0.644003     0.753715      11.41
 O      -0.457557     1.056692     1.858653     220.30
 C       0.031052     2.254494     2.517517     117.21
 H      -0.783307     2.881860     2.803260      25.67
 H       0.482085     1.994869     3.452171      25.88
 H       0.433266     3.042245     1.807858      24.22
 C      -0.453968    -0.248780    -0.162644       7.19
 O      -1.725406    -0.572711     0.264404     187.91
 C       0.360076    -0.861393    -1.241196      55.99
 H      -0.068872    -1.548140    -1.846117      23.04
 C       2.351212     0.393560    -0.599740      31.95
 C       3.907276     0.717862    -0.851619      56.77
 H       4.030000     0.360184    -2.070270      18.69
 O       4.000031     2.194260    -0.969950     222.06
 H       4.390250     2.618538    -0.140257      25.38
 C       4.937104     0.004363     0.139678      92.84
 H       4.582046    -0.000308     1.255073      22.93
 O       4.712296    -1.473491    -0.240092     339.61
 H       5.086960    -1.538220    -1.172008      25.58
 C       6.420762     0.338522    -0.115001     118.86
 O       6.956346     1.748023     0.113039     241.51
 H       7.096066     1.713888     1.103563      29.15
 H       6.586900     0.191131    -1.158400      34.25
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 H       7.077275    -0.322477     0.342466      31.42
55
name= lig-ACN-Water-frame_289
 C      -3.940559     0.426979    -2.836655      40.53
 H      -3.765289    -0.530684    -3.484842      23.89
 C      -3.834203     1.986628    -0.923674      56.62
 H      -3.707290     2.224236     0.175407      25.60
 C      -3.751605     3.137747    -1.827270       2.69
 O      -3.736160     4.491185    -1.571095     169.64
 C      -3.499742     5.039185    -0.129855     114.23
 H      -2.508996     5.267795    -0.168266      27.80
 H      -3.987625     4.267698     0.656290      23.66
 H      -4.267609     5.764861    -0.163774      26.96
 C      -3.816359     2.856884    -3.221221      21.60
 O      -3.651926     3.775136    -4.304661     184.83
 H      -3.841250     4.679263    -4.114613      23.75
 C      -3.890208     1.557946    -3.720332      45.15
 H      -3.657989     1.271373    -4.785140      23.89
 C      -3.834887     0.651396    -1.432635       3.79
 C      -3.980321    -0.628309    -0.569289      79.75
 H      -4.538961    -1.341573    -1.139408      24.73
 O      -4.612559    -0.359168     0.726315     177.79
 H      -3.972426    -0.119693     1.429766      25.79
 C      -2.652366    -1.392120    -0.445976      89.00
 H      -2.191706    -1.452821    -1.497188      25.70
 C      -2.786481    -2.703545     0.272223     110.56
 O      -3.877992    -3.483451    -0.536543     121.97
 H      -3.627354    -3.704233    -1.467120      30.76
 H      -3.202267    -2.784125     1.294008      26.11
 H      -1.897194    -3.236309     0.181912      27.94
 C       1.709014    -0.356208    -1.437249      46.29
 H       2.248850    -0.741226    -2.288015      23.89
 C       1.677689     0.925650     0.530438      99.37
 H       1.983854     1.477504     1.517815      20.14
 C       0.251833     0.575234     0.788266       1.53
 O      -0.439650     1.048898     1.900224     212.28
 C       0.012211     2.322879     2.474275     101.45
 H      -0.949854     2.801125     2.787176      23.82
 H       0.637518     2.155314     3.297782      26.86
 H       0.807434     2.720160     1.803251      23.77
 C      -0.377634    -0.208107    -0.159019      17.61
 O      -1.700288    -0.486329     0.294189     153.69
 C       0.301203    -0.780258    -1.244834      64.68
 H      -0.090003    -1.544063    -1.766052      23.83
 C       2.430232     0.363645    -0.489513      38.23
 C       3.827981     0.732017    -0.872028      72.13
 H       4.172733     0.181216    -1.915176      22.15
 O       4.027310     2.221956    -0.999071     210.25
 H       4.381669     2.421595    -0.145427      27.73
 C       4.913244    -0.011519     0.039476     114.57
 H       4.699051     0.300472     1.118609      24.35
 O       4.766675    -1.443913    -0.141928     311.33
 H       5.178933    -1.862933    -0.917207      28.60
 C       6.459105     0.316467    -0.232014     110.95
 O       6.998181     1.649000     0.094287     253.38
 H       7.049371     1.892041     1.018196      30.21
 H       6.608353     0.234697    -1.257830      32.80
 H       6.948507    -0.419531     0.283834      33.08
55
name= lig-ACN-Water-frame_290
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 C      -3.920128     0.486959    -2.767188      60.51
 H      -4.155956    -0.609085    -2.966462      26.44
 C      -3.833537     2.038964    -0.958882      81.70
 H      -3.739761     2.123697     0.090550      27.14
 C      -3.790039     3.099200    -1.857410      16.26
 O      -3.709574     4.465940    -1.527369     235.88
 C      -3.652725     4.951939    -0.208030     133.61
 H      -2.684471     5.255428     0.149571      28.94
 H      -3.838912     4.226174     0.752481      24.63
 H      -4.093992     5.820274    -0.097101      29.53
 C      -3.788593     2.824951    -3.279213      14.26
 O      -3.681255     3.800365    -4.228251     118.49
 H      -3.965925     4.638938    -3.888995      24.30
 C      -3.846273     1.495636    -3.689005      62.11
 H      -4.141391     1.405710    -4.803702      21.42
 C      -3.822901     0.727762    -1.430104      18.34
 C      -3.993580    -0.570940    -0.607817      83.70
 H      -4.736603    -1.120994    -1.040873      26.34
 O      -4.601478    -0.362180     0.668999     149.23
 H      -3.891325    -0.286353     1.387658      25.93
 C      -2.569452    -1.267522    -0.443102      88.84
 H      -2.160697    -1.583384    -1.497536      26.10
 C      -2.844633    -2.723514     0.259458     103.65
 O      -3.874930    -3.516480    -0.501326     151.68
 H      -3.339665    -3.531324    -1.401705      29.74
 H      -3.259887    -2.485533     1.294265      25.98
 H      -1.917574    -3.245866     0.305096      27.86
 C       1.645860    -0.364928    -1.407332      49.87
 H       2.063981    -0.654321    -2.323049      22.80
 C       1.658767     0.924147     0.658384      70.70
 H       2.432371     1.523210     1.335831      18.74
 C       0.370179     0.615574     0.804765      19.01
 O      -0.406801     1.034940     1.903177     226.28
 C       0.034401     2.350715     2.468020     112.13
 H      -0.889458     3.053006     2.644644      24.67
 H       0.507682     2.243408     3.348109      27.68
 H       0.426685     3.036741     1.683508      25.59
 C      -0.385508    -0.271671    -0.089162      20.88
 O      -1.697072    -0.447099     0.307035     195.70
 C       0.301087    -0.663071    -1.238964      71.60
 H      -0.153873    -1.133419    -2.088528      23.74
 C       2.397329     0.412561    -0.476076      44.07
 C       3.872929     0.741038    -0.873781      78.84
 H       3.830763     0.538470    -2.047495      22.87
 O       4.060536     2.167839    -0.992683     233.64
 H       4.252366     2.694679    -0.161789      27.46
 C       4.953188     0.025789    -0.063535     104.49
 H       4.756301     0.230562     1.007991      23.20
 O       4.818952    -1.416763     0.018389     287.91
 H       4.877818    -1.656692    -0.938577      28.29
 C       6.463187     0.297611    -0.368945     116.69
 O       7.001118     1.548612     0.058819     274.93
 H       6.996927     1.468174     1.019725      32.18
 H       6.743973     0.143298    -1.344626      31.12
 H       6.945712    -0.418993     0.180941      31.82
55
name= lig-ACN-Water-frame_291
 C      -3.911192     0.416485    -2.785287      36.45
 H      -4.264036    -0.541701    -3.165923      22.89
 C      -3.772575     2.097067    -0.898713      65.59
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 H      -3.902343     2.357522     0.060733      21.32
 C      -3.789686     3.108256    -1.878676      14.03
 O      -3.702200     4.439701    -1.541868     245.89
 C      -3.716221     4.889442    -0.152413     121.74
 H      -2.650956     4.982548     0.060094      25.43
 H      -4.362287     4.046566     0.364078      23.22
 H      -4.350595     5.602299    -0.105262      27.04
 C      -3.738515     2.820762    -3.288725      17.95
 O      -3.727564     3.886858    -4.182675     100.86
 H      -3.936499     4.817972    -3.710684      22.59
 C      -3.869579     1.493105    -3.785536      45.93
 H      -4.145825     1.232021    -4.876268      21.80
 C      -3.907418     0.740207    -1.375752      21.12
 C      -3.929549    -0.477685    -0.579440     110.79
 H      -4.370009    -1.157195    -1.174255      27.66
 O      -4.597658    -0.345566     0.693201     230.42
 H      -3.942973    -0.303101     1.450913      24.36
 C      -2.632512    -1.315292    -0.483748      74.33
 H      -2.189971    -1.399680    -1.573174      23.66
 C      -2.891574    -2.679453     0.241407     115.90
 O      -3.767355    -3.498074    -0.484131     209.73
 H      -3.485086    -3.764675    -1.349036      31.35
 H      -3.430055    -2.510656     1.245664      25.39
 H      -1.949929    -3.230731     0.505205      26.42
 C       1.621972    -0.336339    -1.434350      48.18
 H       2.131500    -0.597732    -2.313685      20.18
 C       1.838821     0.901667     0.717122      59.34
 H       2.242804     1.672176     1.470441      14.25
 C       0.379790     0.605233     0.906386      10.22
 O      -0.362038     1.101126     1.941528     231.49
 C      -0.025457     2.411303     2.436364     108.82
 H      -1.086628     2.725044     2.866464      21.67
 H       0.604391     2.323637     3.221762      27.22
 H       0.595779     2.916223     1.692173      25.33
 C      -0.337511    -0.236564     0.025815       7.28
 O      -1.709072    -0.434453     0.326740     157.36
 C       0.230390    -0.600850    -1.265917      57.65
 H      -0.462253    -0.948540    -2.139705      20.20
 C       2.358376     0.443990    -0.528221      24.56
 C       3.825499     0.742190    -0.934058      84.06
 H       4.052530     0.265848    -1.952467      24.32
 O       4.098426     2.182685    -0.986474     201.12
 H       4.178844     2.403694     0.021731      25.41
 C       5.019539     0.063826    -0.031752      90.06
 H       4.997493     0.573635     0.905458      27.10
 O       4.826842    -1.411061     0.093012     277.17
 H       4.771484    -1.906926    -0.786419      27.63
 C       6.489728     0.201535    -0.490676     106.96
 O       6.991980     1.501288    -0.005009     222.34
 H       7.267852     1.649818     0.970224      28.12
 H       6.560971     0.223257    -1.529680      32.65
 H       6.998796    -0.633876    -0.130245      33.37
55
name= lig-ACN-Water-frame_292
 C      -3.975326     0.491671    -2.849745      61.39
 H      -3.891873    -0.498863    -3.167233      24.94
 C      -3.780307     2.051096    -0.914680      63.19
 H      -3.680541     2.147687     0.106993      22.30
 C      -3.703539     3.100034    -1.888415       9.07
 O      -3.715310     4.478517    -1.621245     188.96
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 C      -3.833996     4.763115    -0.123972     123.11
 H      -2.893400     4.905085     0.488760      27.49
 H      -4.367107     4.088264     0.614250      26.82
 H      -4.105933     5.703769    -0.113692      28.11
 C      -3.746748     2.842844    -3.294529      13.99
 O      -3.764121     3.954041    -4.178295     146.32
 H      -4.016445     4.902149    -3.747721      21.51
 C      -3.896401     1.507320    -3.776453      57.07
 H      -3.687226     1.289713    -4.842012      22.84
 C      -3.917933     0.774624    -1.455787      21.36
 C      -3.950273    -0.547966    -0.514964      86.90
 H      -4.663603    -1.128594    -0.881514      26.62
 O      -4.601852    -0.329830     0.762145     178.26
 H      -3.975035    -0.130585     1.486092      25.05
 C      -2.621250    -1.272586    -0.449493      92.59
 H      -2.251601    -1.523914    -1.524697      25.18
 C      -2.841598    -2.596505     0.279648     100.33
 O      -3.736556    -3.534305    -0.531461     166.51
 H      -3.132602    -3.766263    -1.251782      31.37
 H      -3.478227    -2.418404     1.223977      25.33
 H      -1.772086    -2.996141     0.463545      25.80
 C       1.574971    -0.239244    -1.486962      50.24
 H       1.902082    -0.613256    -2.458060      23.55
 C       1.787866     0.865292     0.691088      92.28
 H       2.440158     1.392466     1.364840      24.64
 C       0.493676     0.556637     0.991510       7.67
 O      -0.345968     1.133701     2.008322     224.44
 C      -0.033930     2.468266     2.477841     107.01
 H      -0.999289     3.095208     2.848604      24.23
 H       0.689272     2.508350     3.215827      27.28
 H       0.128318     3.163359     1.671099      26.37
 C      -0.347051    -0.203007    -0.004411      20.58
 O      -1.670845    -0.452638     0.360489     168.04
 C       0.191612    -0.517957    -1.182447      56.58
 H      -0.455578    -1.225534    -1.975576      20.36
 C       2.434147     0.415644    -0.555307      33.90
 C       3.904116     0.678517    -0.936630      82.50
 H       4.007030     0.428451    -2.004288      25.15
 O       4.106783     2.173552    -0.964647     195.61
 H       4.420770     2.540988    -0.123512      28.99
 C       5.006384    -0.008013    -0.007728     109.82
 H       4.912898     0.270652     0.996155      27.83
 O       4.777527    -1.390065     0.175444     287.78
 H       5.123860    -1.727941    -0.694854      27.50
 C       6.487901     0.213709    -0.597683     108.67
 O       7.042395     1.490054    -0.146267     206.23
 H       7.154673     1.339608     0.871104      28.66
 H       6.464333     0.327820    -1.662885      30.22
 H       7.164233    -0.575260    -0.336214      32.15
55
name= lig-ACN-Water-frame_293
 C      -3.993081     0.496549    -2.861749      50.40
 H      -3.910847    -0.486787    -3.189626      26.17
 C      -3.774013     2.014060    -1.023708      56.84
 H      -3.539024     2.176187     0.043152      22.69
 C      -3.659673     3.119364    -1.892836      11.61
 O      -3.720854     4.485238    -1.519577     224.32
 C      -3.896647     4.755050    -0.143170     115.04
 H      -2.912193     4.327859     0.245475      26.50
 H      -4.760166     4.135078     0.056746      27.84
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 H      -4.250915     5.728606     0.056065      26.59
 C      -3.813068     2.940528    -3.316297      14.15
 O      -3.780085     3.946287    -4.201161     157.08
 H      -4.216591     4.685148    -3.772892      26.18
 C      -3.829946     1.641525    -3.808920      53.34
 H      -3.811574     1.506507    -4.869708      23.61
 C      -3.926959     0.639965    -1.451873      14.21
 C      -4.085775    -0.494967    -0.534843      87.71
 H      -4.554042    -1.213704    -1.038325      26.36
 O      -4.585580    -0.282889     0.858968     201.86
 H      -3.848626    -0.042458     1.469773      24.09
 C      -2.592357    -1.222900    -0.387470      78.99
 H      -2.178867    -1.374318    -1.433720      25.51
 C      -2.812375    -2.604010     0.313550     100.23
 O      -3.619928    -3.525228    -0.558215     136.83
 H      -2.973193    -3.845476    -1.325938      27.26
 H      -3.279472    -2.443655     1.350863      25.08
 H      -1.837990    -3.260742     0.532431      24.78
 C       1.537300    -0.159896    -1.540115      52.06
 H       1.994601    -0.463021    -2.536317      24.79
 C       1.835864     0.807954     0.634721      90.58
 H       2.404784     1.256261     1.342521      25.03
 C       0.403561     0.555798     0.991234       9.60
 O      -0.302149     1.119544     2.090291     204.99
 C      -0.024953     2.608118     2.492330      82.20
 H      -0.975630     2.662251     3.131788      23.85
 H       0.819044     2.671771     3.142636      25.88
 H       0.183486     3.106955     1.547917      26.84
 C      -0.368183    -0.123783     0.075319      23.58
 O      -1.653978    -0.477984     0.413960     188.74
 C       0.267109    -0.504542    -1.189724      59.38
 H      -0.311343    -1.276700    -2.036630      20.41
 C       2.425143     0.349801    -0.566129      30.91
 C       3.953470     0.686841    -0.875785      89.34
 H       4.131631     0.320240    -1.862319      25.19
 O       4.124399     2.125654    -0.946358     210.09
 H       4.519758     2.427536    -0.119107      28.79
 C       5.024572    -0.025105    -0.000328     106.18
 H       4.965847     0.475767     0.909766      29.85
 O       4.740367    -1.459694     0.180384     287.23
 H       5.007718    -2.026394    -0.552613      28.56
 C       6.411144     0.279097    -0.681730     104.45
 O       7.102024     1.481684    -0.272017     196.60
 H       7.367985     1.516487     0.680759      30.11
 H       6.301866     0.269462    -1.796409      29.55
 H       7.030201    -0.594895    -0.425859      30.77
55
name= lig-ACN-Water-frame_294
 C      -3.932796     0.497797    -2.967196      51.05
 H      -4.359327    -0.300300    -3.517851      22.72
 C      -3.711005     2.004761    -1.057214      58.03
 H      -3.818646     2.229186     0.087295      19.42
 C      -3.735515     3.163672    -1.913032      19.90
 O      -3.688891     4.477003    -1.510528     213.51
 C      -4.000228     4.668178    -0.092075     123.69
 H      -3.374178     4.313735     0.788565      24.98
 H      -4.934778     4.328780     0.248184      27.10
 H      -3.782815     5.769461    -0.029769      25.35
 C      -3.814427     2.955216    -3.276891      14.33
 O      -3.817055     4.009924    -4.268219     148.80
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 H      -4.081493     4.878746    -4.063085      26.21
 C      -3.807050     1.610420    -3.758826      49.34
 H      -4.069834     1.469763    -4.753977      23.94
 C      -3.982500     0.728394    -1.517571      10.05
 C      -4.001936    -0.547590    -0.452287      85.78
 H      -4.712183    -1.208905    -0.765066      25.71
 O      -4.591109    -0.212024     0.840308     223.96
 H      -3.862761    -0.201381     1.552397      22.92
 C      -2.633910    -1.240469    -0.344391      89.90
 H      -2.239068    -1.299684    -1.356241      24.76
 C      -2.757510    -2.679104     0.301054     100.84
 O      -3.497078    -3.489479    -0.568036     218.43
 H      -2.937883    -3.707250    -1.330647      30.38
 H      -3.475996    -2.694002     1.185692      24.44
 H      -1.593806    -2.942032     0.539618      23.70
 C       1.628683    -0.149089    -1.566916      30.83
 H       1.962479    -0.379697    -2.661060      19.67
 C       1.787823     0.741330     0.714674      53.09
 H       2.348937     1.244356     1.386121      16.31
 C       0.427096     0.702614     0.955214      20.50
 O      -0.177192     1.122168     2.174575     249.23
 C      -0.006996     2.557227     2.478375     115.18
 H      -0.783492     3.025218     3.133003      23.35
 H       1.016667     2.746271     2.928903      23.96
 H      -0.184292     3.253648     1.662307      25.88
 C      -0.343032    -0.155956    -0.003525      23.01
 O      -1.690879    -0.466265     0.512621     153.18
 C       0.231544    -0.528113    -1.187711      57.29
 H      -0.579097    -1.000851    -2.063634      17.56
 C       2.418727     0.378851    -0.554150      33.96
 C       3.852665     0.625337    -0.868755      87.45
 H       4.022583     0.293548    -1.839645      25.28
 O       4.176567     2.077425    -0.902526     209.91
 H       4.305922     2.384221     0.085271      24.95
 C       5.018249     0.003120     0.003109      97.41
 H       5.160662     0.154393     1.026894      25.57
 O       4.737951    -1.502413     0.175754     319.65
 H       4.802792    -1.744607    -0.778627      26.06
 C       6.376172     0.230497    -0.713297      99.23
 O       7.121391     1.502939    -0.357749     177.13
 H       7.428574     1.364983     0.531952      34.14
 H       6.217386     0.471702    -1.827854      31.87
 H       7.060521    -0.670498    -0.580481      31.35
55
name= lig-ACN-Water-frame_295
 C      -3.964364     0.494045    -2.926939      53.56
 H      -4.241449    -0.557543    -3.211646      22.88
 C      -3.753121     2.053558    -1.051482      50.98
 H      -3.757983     2.082350     0.146985      17.86
 C      -3.790405     3.151379    -1.904792      16.15
 O      -3.655546     4.454264    -1.430007     209.13
 C      -4.090369     4.702488     0.025004     103.65
 H      -3.456455     3.932265     0.531792      22.63
 H      -5.081060     4.703698     0.055072      26.92
 H      -3.821943     5.853516     0.222261      23.03
 C      -3.769858     3.001033    -3.385308      16.95
 O      -3.843091     4.001815    -4.324537     162.44
 H      -4.085748     4.840016    -3.788710      23.32
 C      -3.875368     1.668124    -3.826364      54.14
 H      -3.842997     1.539619    -4.889995      21.99
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 C      -3.927781     0.691986    -1.549162      16.88
 C      -3.981914    -0.498387    -0.449957      88.80
 H      -4.493892    -1.277856    -0.989145      25.17
 O      -4.593055    -0.124095     0.811424     235.28
 H      -3.967547    -0.064792     1.622968      20.80
 C      -2.626238    -1.269585    -0.281269      89.88
 H      -2.279773    -1.447023    -1.266194      23.98
 C      -2.702074    -2.636276     0.320298     104.14
 O      -3.397193    -3.544351    -0.659179     217.40
 H      -2.889628    -3.507818    -1.454385      31.27
 H      -3.137821    -2.593893     1.369439      23.86
 H      -1.630032    -3.191571     0.514196      22.83
 C       1.531885    -0.222932    -1.495553      29.86
 H       2.050307    -0.399823    -2.524977      15.45
 C       1.820455     0.782326     0.750232      26.26
 H       2.464922     1.106698     1.544742      12.06
 C       0.406833     0.689486     0.916072      22.45
 O      -0.058748     1.128207     2.191026     239.03
 C       0.029925     2.543662     2.458196      99.91
 H      -0.549421     2.570099     3.324818      23.43
 H       1.108277     2.879348     2.713283      22.94
 H      -0.299492     3.013193     1.492090      22.81
 C      -0.385920    -0.110820     0.063736      18.99
 O      -1.649482    -0.433181     0.507632     157.35
 C       0.214096    -0.490956    -1.255181      68.22
 H      -0.420711    -1.052055    -2.177323      18.87
 C       2.351668     0.406706    -0.484152      24.28
 C       3.861512     0.634245    -0.814751      85.98
 H       3.960198     0.358111    -1.778680      23.91
 O       4.188322     2.049481    -0.839174     215.06
 H       4.313579     2.376361     0.143369      23.95
 C       4.986605    -0.116328     0.034018      88.08
 H       4.824072     0.434777     0.940782      25.06
 O       4.770238    -1.461941     0.109995     322.52
 H       4.988303    -1.973972    -0.748168      25.60
 C       6.392400     0.250636    -0.775006      85.54
 O       7.084476     1.441275    -0.390005     205.23
 H       7.281792     1.510025     0.603318      32.82
 H       6.122772     0.243704    -1.914291      29.38
 H       7.111417    -0.676645    -0.620523      29.89
55
name= lig-ACN-Water-frame_296
 C      -4.015913     0.565912    -2.916514      42.81
 H      -3.732139    -0.412282    -3.462750      22.95
 C      -3.856289     2.006287    -1.070070      47.99
 H      -3.640424     2.353709     0.028825      19.73
 C      -3.775624     3.161137    -1.938854       9.26
 O      -3.658989     4.485566    -1.317335     231.92
 C      -4.135666     4.732173    -0.001188     119.87
 H      -3.972901     4.042451     0.860710      25.29
 H      -5.111957     4.734661     0.047215      27.90
 H      -3.582955     5.701478     0.528167      24.74
 C      -3.800182     2.954490    -3.350380      11.59
 O      -3.847797     3.991437    -4.323407     127.42
 H      -4.084483     5.028928    -4.057967      21.36
 C      -3.928765     1.598225    -3.865287      43.87
 H      -3.829683     1.388265    -4.956520      22.72
 C      -3.821277     0.709210    -1.457660      17.77
 C      -3.949051    -0.448245    -0.528612      72.77
 H      -4.709615    -1.171252    -0.878236      22.28
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 O      -4.625330    -0.042193     0.753455     214.91
 H      -3.897070     0.033478     1.413384      23.42
 C      -2.528944    -1.193091    -0.302898      94.90
 H      -2.114135    -1.290529    -1.258823      24.80
 C      -2.651674    -2.696329     0.338415      91.69
 O      -3.316807    -3.575675    -0.700024     163.30
 H      -2.764203    -3.426007    -1.575562      27.57
 H      -3.329650    -2.888481     1.202721      23.37
 H      -1.470965    -2.981165     0.432103      22.39
 C       1.536274    -0.223843    -1.373231      59.33
 H       1.931566    -0.700152    -2.330703      21.14
 C       1.813925     0.837851     0.708354     105.22
 H       2.418912     1.250713     1.596175      18.11
 C       0.477197     0.608150     0.983057      12.54
 O       0.002205     1.045528     2.187056     235.97
 C       0.065178     2.528064     2.424215      95.38
 H      -0.352831     2.741146     3.337099      24.79
 H       1.188768     2.951587     2.431603      21.74
 H      -0.603865     3.194409     1.833704      24.76
 C      -0.373237    -0.054307     0.002534      23.56
 O      -1.652150    -0.401854     0.480421     186.37
 C       0.084667    -0.439200    -1.191462      80.42
 H      -0.470715    -1.155864    -1.935753      19.30
 C       2.395857     0.380086    -0.475631      44.85
 C       3.852906     0.633550    -0.823665      93.38
 H       3.972150     0.344330    -1.770859      25.70
 O       4.161034     2.070624    -0.768295     193.49
 H       4.576938     2.281864     0.120027      24.21
 C       4.973667    -0.050048    -0.057124     127.56
 H       5.201673     0.043982     1.014728      21.37
 O       4.800206    -1.536693     0.101685     287.20
 H       5.132158    -1.889901    -0.804652      24.14
 C       6.342479     0.187405    -0.729030      90.91
 O       7.042048     1.423612    -0.420157     177.29
 H       7.097823     1.423478     0.627056      30.74
 H       6.227186     0.356664    -1.874452      29.91
 H       7.059145    -0.751660    -0.504352      31.07
55
name= lig-ACN-Water-frame_297
 C      -3.895387     0.531393    -2.913281      58.75
 H      -4.001158    -0.613434    -3.245430      23.68
 C      -3.849730     2.113661    -1.031831      60.59
 H      -3.959519     2.148126     0.068796      20.67
 C      -3.783009     3.195316    -1.881446      13.53
 O      -3.634503     4.462952    -1.322406     214.47
 C      -4.241589     4.724366     0.056777     103.59
 H      -3.975100     3.912597     0.700587      26.11
 H      -5.117262     5.106936    -0.026446      27.38
 H      -3.588630     5.777111     0.127933      23.92
 C      -3.924366     2.986801    -3.336813      13.75
 O      -3.827814     3.951178    -4.314316      16.19
 H      -4.119528     4.833547    -3.885541      23.82
 C      -3.939404     1.649904    -3.764110      56.50
 H      -4.126604     1.403546    -4.867590      21.24
 C      -3.856969     0.766907    -1.573002       4.83
 C      -3.897488    -0.455983    -0.503141      73.45
 H      -4.500326    -1.275665    -1.093288      24.17
 O      -4.609587     0.015249     0.657156     191.98
 H      -4.123629     0.108560     1.489276      23.28
 C      -2.570552    -1.198161    -0.339634      87.41
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 H      -2.197533    -1.341724    -1.329715      25.15
 C      -2.623886    -2.713018     0.204396     115.27
 O      -3.209578    -3.564818    -0.722059     226.20
 H      -2.651721    -3.623579    -1.580837      26.91
 H      -3.232201    -2.614504     1.120036      24.43
 H      -1.586425    -3.120156     0.664521      22.98
 C       1.517912    -0.298932    -1.407261      47.43
 H       1.972674    -0.775411    -2.281457      24.00
 C       1.859179     0.864271     0.697562      81.86
 H       2.505893     1.612325     1.371918      15.93
 C       0.521091     0.567956     1.008581      12.28
 O      -0.026592     1.023889     2.255269     258.96
 C       0.068981     2.493216     2.441785      78.52
 H       0.013601     2.623699     3.445525      23.74
 H       1.159999     2.816021     2.020305      19.94
 H      -0.688589     2.878975     1.700562      23.93
 C      -0.411740     0.007809     0.100042      19.27
 O      -1.683368    -0.314673     0.513981     164.08
 C       0.174811    -0.429375    -1.166719      62.40
 H      -0.432953    -0.969915    -1.869506      20.88
 C       2.433458     0.359200    -0.475365      48.03
 C       3.869880     0.646200    -0.860173      89.09
 H       3.973764     0.429625    -1.811691      22.13
 O       4.106661     2.107364    -0.750046     211.41
 H       4.392344     2.285162     0.168361      23.38
 C       5.032841    -0.115146    -0.025820     112.51
 H       4.912926     0.474854     0.909883      21.72
 O       4.822151    -1.595738     0.084752     300.20
 H       4.781698    -1.921372    -0.870960      24.43
 C       6.346366     0.143657    -0.750552      87.71
 O       6.990849     1.427134    -0.410758     231.27
 H       7.298986     1.439670     0.586160      31.89
 H       6.245238     0.006238    -1.876040      30.40
 H       7.032762    -0.785944    -0.344305      28.70
55
name= lig-ACN-Water-frame_298
 C      -3.789145     0.504312    -2.923802      46.79
 H      -4.193426    -0.524974    -3.352213      21.96
 C      -3.843406     2.055397    -1.008774      65.63
 H      -3.970770     2.190889    -0.001734      21.16
 C      -3.852009     3.210413    -1.851452      17.63
 O      -3.651360     4.494962    -1.352681     238.21
 C      -4.244486     4.816492    -0.023296     117.67
 H      -4.190545     4.036699     0.678945      26.76
 H      -5.207778     4.855489    -0.098643      27.25
 H      -3.691780     5.654299     0.701657      24.23
 C      -3.955443     2.998058    -3.226694      23.10
 O      -3.836970     3.965417    -4.273421     156.18
 H      -4.060389     4.821361    -4.027554      27.16
 C      -3.981197     1.655262    -3.739121      22.79
 H      -4.126726     1.713000    -4.875566      22.41
 C      -3.874923     0.761413    -1.494786      15.45
 C      -3.901098    -0.405653    -0.586142      82.70
 H      -4.625907    -1.234304    -1.003952      23.26
 O      -4.612475     0.027294     0.605064     215.79
 H      -3.879526     0.011773     1.285563      25.04
 C      -2.541718    -1.177543    -0.368732      84.58
 H      -2.068885    -1.118223    -1.367423      21.35
 C      -2.607601    -2.583401     0.207434     108.81
 O      -3.149564    -3.597752    -0.803546     225.32
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 H      -2.462518    -3.677870    -1.428627      30.67
 H      -3.314967    -2.730817     1.010764      24.56
 H      -1.511818    -2.901644     0.417390      22.55
 C       1.641427    -0.368143    -1.436273      36.51
 H       1.920784    -0.605344    -2.432424      14.20
 C       1.880320     0.855068     0.674498      55.97
 H       2.568148     1.512852     1.400464      16.70
 C       0.488223     0.636683     1.094020       8.17
 O      -0.034930     0.984798     2.323297     276.52
 C       0.069639     2.417107     2.420138      99.26
 H       0.089130     2.749015     3.415055      23.44
 H       1.053584     2.931190     1.893637      21.26
 H      -0.869763     2.966410     2.127383      23.13
 C      -0.330193    -0.050357     0.142921       9.03
 O      -1.724461    -0.248198     0.505073     184.02
 C       0.191541    -0.446891    -1.100590      65.84
 H      -0.362132    -0.754469    -1.859290      22.53
 C       2.415521     0.318960    -0.534238      42.09
 C       3.906938     0.648492    -0.896848      87.35
 H       4.065629     0.466382    -1.831719      23.54
 O       4.033759     2.121331    -0.784549     192.33
 H       4.380252     2.395428     0.062700      25.01
 C       4.969927    -0.180510    -0.047780      94.03
 H       5.032822    -0.026714     1.077400      23.81
 O       4.794651    -1.562054     0.085926     312.47
 H       5.104157    -2.033694    -0.784844      26.76
 C       6.458706     0.101033    -0.688217      92.42
 O       6.952146     1.412732    -0.460814     262.58
 H       7.028047     1.496603     0.546368      30.68
 H       6.350868     0.076373    -1.791050      31.41
 H       7.320491    -0.729798    -0.366547      29.13
55
name= lig-ACN-Water-frame_299
 C      -3.866680     0.596529    -2.923089      56.53
 H      -3.593799    -0.412085    -3.418200      23.64
 C      -3.870404     2.034729    -0.964876      52.50
 H      -3.662052     2.136173     0.007250      18.45
 C      -3.902466     3.188285    -1.781947       9.39
 O      -3.675570     4.606322    -1.339384     222.52
 C      -4.287542     4.807133    -0.083393     121.97
 H      -4.045388     4.039448     0.595834      27.19
 H      -5.212855     5.109101    -0.172867      26.62
 H      -3.824750     5.918634     0.137078      22.86
 C      -3.914618     2.994754    -3.240991      27.54
 O      -3.871543     3.997539    -4.194380     150.19
 H      -4.118787     4.874693    -3.793328      24.63
 C      -3.983796     1.689729    -3.745490      58.84
 H      -3.932070     1.385089    -4.811262      25.67
 C      -3.804064     0.732147    -1.560618      26.19
 C      -3.970395    -0.449525    -0.619564      62.05
 H      -4.669243    -1.248154    -1.206399      23.43
 O      -4.576288    -0.020159     0.637393     184.74
 H      -3.968361     0.163632     1.422473      21.84
 C      -2.532399    -1.005195    -0.414622     101.74
 H      -2.082662    -1.328588    -1.410509      23.37
 C      -2.603452    -2.557867     0.163300     102.16
 O      -3.075398    -3.554633    -0.822133     262.41
 H      -2.455449    -3.634569    -1.602930      28.91
 H      -3.173442    -2.591215     1.078777      24.92
 H      -1.574517    -2.757207     0.551483      24.69
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 C       1.587990    -0.374987    -1.431520      40.30
 H       1.959053    -0.671234    -2.384936      15.28
 C       1.845536     0.790247     0.680284      29.92
 H       2.562340     1.164867     1.486283      17.82
 C       0.536956     0.585988     1.051198      27.53
 O      -0.002276     0.972324     2.357316     248.54
 C       0.000145     2.490736     2.512255      76.21
 H       0.325434     2.693068     3.564914      20.86
 H       0.872651     2.798001     1.753453      21.63
 H      -0.986468     2.843930     2.106447      20.89
 C      -0.301558    -0.141319     0.160090      21.61
 O      -1.686414    -0.217158     0.437189     209.68
 C       0.258589    -0.514142    -1.102999      42.11
 H      -0.358448    -0.879980    -1.721778      21.30
 C       2.482341     0.333438    -0.520934      54.47
 C       3.896772     0.631522    -0.884614      93.33
 H       4.021792     0.344810    -1.781558      25.03
 O       3.997145     2.118731    -0.839757     173.12
 H       4.408769     2.313588     0.033662      24.71
 C       5.087278    -0.137071    -0.049468      92.48
 H       5.025415     0.428842     0.927500      23.18
 O       4.719582    -1.619229     0.018890     284.74
 H       5.228682    -2.004836    -0.772965      25.64
 C       6.468847     0.058815    -0.643798     100.43
 O       6.939668     1.448060    -0.497025     315.24
 H       7.105406     1.592783     0.480096      33.37
 H       6.483241    -0.160735    -1.706106      32.50
 H       7.195485    -0.779916    -0.090015      29.04
55
name= lig-ACN-Water-frame_300
 C      -3.898980     0.592954    -2.950999      52.71
 H      -3.638014    -0.413100    -3.316539      21.87
 C      -3.834641     2.093595    -0.955623      53.56
 H      -3.816656     2.091586     0.099264      19.99
 C      -3.860849     3.236925    -1.823371      23.51
 O      -3.723442     4.521229    -1.422467     229.45
 C      -4.347208     4.949882    -0.091675     106.93
 H      -4.064400     4.306050     0.731097      27.05
 H      -5.330725     4.831869    -0.136760      27.03
 H      -3.848340     5.942556     0.250726      24.85
 C      -3.921024     3.028142    -3.231771       9.02
 O      -3.916413     4.084260    -4.102798      52.81
 H      -4.173139     4.999843    -3.573045      21.57
 C      -3.909567     1.722733    -3.831951      52.84
 H      -3.897181     1.784134    -4.906391      26.19
 C      -3.870749     0.806260    -1.533151      24.13
 C      -3.886031    -0.419733    -0.563783      72.56
 H      -4.527405    -1.377939    -0.996796      21.75
 O      -4.570666    -0.109677     0.674936     221.89
 H      -3.834846    -0.035434     1.307105      25.29
 C      -2.545576    -1.135274    -0.453021      82.55
 H      -2.201654    -0.869774    -1.525820      21.24
 C      -2.542049    -2.496117     0.139747     130.59
 O      -3.037283    -3.437295    -0.784924     245.41
 H      -2.464139    -3.341372    -1.677758      25.32
 H      -3.344987    -2.514375     0.854039      23.52
 H      -1.604997    -2.847014     0.476434      26.11
 C       1.619833    -0.306440    -1.410140      46.33
 H       2.027171    -0.817204    -2.288977      23.76
 C       1.940426     0.699023     0.770094      79.98
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 H       2.514787     1.222959     1.511198      18.96
 C       0.507444     0.470789     1.077496      -0.09
 O       0.053888     0.990943     2.309485     234.49
 C      -0.029761     2.484920     2.544320      85.36
 H       0.193288     2.767205     3.654406      21.94
 H       0.658274     3.151705     1.895198      23.63
 H      -1.091463     2.896259     2.480097      22.51
 C      -0.319322    -0.166141     0.110297      15.01
 O      -1.655832    -0.184975     0.347684     177.04
 C       0.228063    -0.645902    -1.104008      87.97
 H      -0.177095    -1.269933    -1.782435      19.20
 C       2.440329     0.284446    -0.488929      30.76
 C       3.938932     0.605324    -0.895905      92.64
 H       4.040080     0.413679    -1.821596      26.01
 O       4.026007     2.091299    -0.891982     152.46
 H       4.139976     2.511308     0.057046      23.14
 C       5.028238    -0.107805    -0.072856     101.17
 H       5.071462     0.011668     1.032925      22.86
 O       4.700119    -1.567796    -0.045381     353.58
 H       4.819839    -1.974324    -0.935840      27.26
 C       6.497068     0.051194    -0.612149     101.25
 O       6.952307     1.459597    -0.532292     276.80
 H       7.246516     1.563930     0.436641      29.28
 H       6.628997    -0.341919    -1.600528      31.39
 H       7.221733    -0.544590     0.161004      27.10
55
name= lig-ACN-Water-frame_301
 C      -3.869722     0.620916    -2.968654      57.92
 H      -4.263374    -0.259390    -3.382563      25.34
 C      -3.825436     2.123676    -0.981952      61.87
 H      -4.009736     2.502099     0.063525      19.20
 C      -3.809310     3.193328    -1.837750      20.09
 O      -3.795606     4.547652    -1.422765     222.44
 C      -4.360467     4.994529    -0.122826     122.55
 H      -3.874056     4.447408     0.738272      25.25
 H      -5.404608     4.961664    -0.176485      27.43
 H      -4.232477     6.040340    -0.077512      26.69
 C      -3.921995     3.050064    -3.254267      14.76
 O      -3.962174     4.200153    -4.044896     107.86
 H      -4.237708     5.157338    -3.727046      19.41
 C      -3.828002     1.771131    -3.822895      57.05
 H      -3.892770     1.598805    -4.862291      24.76
 C      -3.965272     0.821869    -1.499020      16.95
 C      -3.880265    -0.396113    -0.568832      82.00
 H      -4.665984    -1.104538    -1.202272      21.88
 O      -4.505766    -0.194903     0.737719     222.30
 H      -3.995105    -0.109260     1.561442      24.02
 C      -2.458377    -1.050000    -0.507544      88.89
 H      -2.019349    -1.473065    -1.505550      19.90
 C      -2.496937    -2.464466     0.194423     105.58
 O      -3.065797    -3.372707    -0.824083     244.97
 H      -2.458045    -3.486930    -1.650670      26.43
 H      -3.082893    -2.481060     1.104131      24.69
 H      -1.549835    -2.633510     0.567519      26.80
 C       1.612357    -0.383746    -1.390278      40.31
 H       2.043633    -0.574944    -2.419772      23.17
 C       1.955305     0.592920     0.855820      47.66
 H       2.493439     1.140376     1.539776      20.08
 C       0.589047     0.483662     1.090542       5.18
 O       0.055885     1.020520     2.263761     247.59
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 C      -0.074353     2.460587     2.556397      73.91
 H       0.379234     2.496976     3.689071      20.18
 H       0.577343     3.017139     1.881179      25.49
 H      -1.162496     2.663700     2.385855      21.17
 C      -0.303810    -0.169576     0.045509       2.42
 O      -1.705687    -0.185555     0.307306     180.02
 C       0.305498    -0.734739    -1.112440      44.91
 H      -0.346448    -1.347058    -1.768411      15.44
 C       2.497297     0.262313    -0.432718      24.58
 C       3.891859     0.652991    -0.897565      97.93
 H       4.035167     0.326031    -1.789816      27.59
 O       4.075939     2.097469    -0.932869     174.76
 H       4.097266     2.372340     0.052237      26.15
 C       4.980172    -0.174322    -0.079616      99.35
 H       4.836643     0.225003     0.941502      26.15
 O       4.692346    -1.522358    -0.126772     322.66
 H       4.760511    -1.846249    -1.058884      28.63
 C       6.529686     0.092227    -0.522375      94.23
 O       6.990316     1.445760    -0.576911     278.89
 H       7.087638     1.752443     0.381360      29.90
 H       6.643564    -0.214476    -1.554796      29.85
 H       7.184409    -0.646781     0.147588      27.34
55
name= lig-ACN-Water-frame_302
 C      -3.946606     0.717255    -2.870538      51.82
 H      -4.083256    -0.206590    -3.302551      23.86
 C      -3.887209     2.141644    -0.969058      46.04
 H      -3.750093     2.003286     0.209684      17.33
 C      -3.824262     3.289345    -1.849362      18.93
 O      -3.847072     4.618892    -1.421285     250.20
 C      -4.394976     4.993778    -0.192320     128.30
 H      -3.838486     4.620647     0.738214      28.31
 H      -5.409286     4.705618    -0.004870      28.50
 H      -4.151169     5.940855    -0.186931      27.97
 C      -3.846073     3.169162    -3.288032       1.06
 O      -3.990487     4.246225    -4.094355     155.20
 H      -4.345996     4.885767    -3.537569      26.08
 C      -3.802024     1.793020    -3.771620      52.14
 H      -3.881675     1.602404    -4.819766      25.90
 C      -3.924004     0.820208    -1.520960      36.59
 C      -3.943537    -0.422182    -0.627222      77.42
 H      -4.529560    -1.451416    -0.981891      21.44
 O      -4.439241    -0.241081     0.786778     204.93
 H      -3.563187    -0.066451     1.265470      23.51
 C      -2.504417    -1.046605    -0.482391      72.74
 H      -2.103941    -0.938241    -1.576382      21.42
 C      -2.473215    -2.438058     0.195012     125.59
 O      -3.122260    -3.347727    -0.788320     254.97
 H      -2.433380    -3.550325    -1.379850      29.64
 H      -3.124005    -2.503265     1.066121      24.22
 H      -1.564641    -2.833750     0.294763      27.89
 C       1.706235    -0.462731    -1.351338      32.09
 H       2.076030    -0.608860    -2.428023      14.62
 C       2.001721     0.548800     0.851199      27.78
 H       2.659876     0.819801     1.636290      14.96
 C       0.541199     0.504397     1.007855      18.81
 O      -0.002914     0.952443     2.236346     227.64
 C      -0.069319     2.393652     2.504466      94.30
 H       0.208820     2.731214     3.657666      21.56
 H       0.530695     2.967599     1.862587      26.03
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 H      -1.098745     2.860612     2.441987      21.05
 C      -0.248439    -0.145810     0.107522      24.86
 O      -1.607552    -0.132384     0.282550     204.64
 C       0.347604    -0.719720    -1.049799      75.63
 H      -0.236858    -1.129801    -2.021179      16.20
 C       2.495745     0.219977    -0.448669      30.22
 C       3.886790     0.633654    -0.933754      87.51
 H       3.875783     0.461938    -1.895983      26.08
 O       4.104337     2.120015    -0.943547     214.35
 H       4.332149     2.505088    -0.090799      25.81
 C       5.016636    -0.044646    -0.068892      89.97
 H       4.904409     0.091019     0.994435      23.89
 O       4.675561    -1.565337    -0.206716     302.09
 H       5.179684    -1.899400    -1.029862      27.91
 C       6.463928     0.084730    -0.501550     108.16
 O       7.036625     1.471282    -0.567350     277.64
 H       7.164024     1.715579     0.382512      32.37
 H       6.544484    -0.397069    -1.494106      32.33
 H       7.153972    -0.504740     0.203039      28.86
55
name= lig-ACN-Water-frame_303
 C      -3.997690     0.715312    -2.923561      52.90
 H      -3.738553    -0.208608    -3.313498      26.15
 C      -3.897281     2.179899    -0.966025      56.44
 H      -3.787130     2.587692     0.180441      17.38
 C      -3.879729     3.309505    -1.806675      16.89
 O      -3.872858     4.667416    -1.496126     223.65
 C      -4.406510     4.984482    -0.113157     111.91
 H      -3.737147     4.409591     0.589720      25.40
 H      -5.437203     4.608486    -0.151547      27.31
 H      -4.382779     5.984693     0.155346      25.62
 C      -3.779421     3.144440    -3.208945      15.57
 O      -3.998627     4.240895    -4.168027     174.60
 H      -4.131244     5.171107    -3.898947      25.39
 C      -3.844694     1.893004    -3.747683      44.49
 H      -3.813911     1.818661    -4.848945      23.84
 C      -3.935318     0.863358    -1.438273       3.28
 C      -3.908469    -0.471009    -0.521217      80.31
 H      -4.700581    -1.144108    -1.195949      21.50
 O      -4.346101    -0.234858     0.762248     269.49
 H      -3.689555     0.043756     1.455625      23.23
 C      -2.491168    -1.012027    -0.490512      88.04
 H      -2.120698    -1.183764    -1.567317      23.93
 C      -2.481916    -2.444786     0.100908     125.84
 O      -3.192124    -3.361155    -0.714045     244.26
 H      -2.735341    -3.568330    -1.572264      29.18
 H      -2.996624    -2.344930     1.066087      25.27
 H      -1.532651    -2.640910     0.429360      28.74
 C       1.752625    -0.500875    -1.338998      41.82
 H       2.168763    -1.052442    -2.238045      18.94
 C       1.989705     0.542053     0.797311      66.43
 H       2.628509     0.938475     1.661211      18.47
 C       0.601922     0.529722     1.068090       3.60
 O      -0.087823     0.881821     2.231324     238.11
 C      -0.066977     2.388599     2.417404      86.15
 H       0.355798     2.440278     3.587662      19.94
 H       0.661959     2.770641     1.799280      26.27
 H      -1.110159     2.648298     2.223712      21.18
 C      -0.211540    -0.172166     0.051086      13.61
 O      -1.600357    -0.057481     0.302635     164.38
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 C       0.387195    -0.642372    -1.073518      51.99
 H      -0.381283    -1.268794    -1.833868      18.14
 C       2.564257     0.205394    -0.450516      31.42
 C       3.961261     0.684341    -0.914628      91.93
 H       4.202773     0.264835    -1.807385      26.13
 O       4.089091     2.137366    -0.963691     255.31
 H       4.318552     2.421564    -0.076301      25.73
 C       4.992692    -0.090433    -0.096991     111.60
 H       4.883748     0.196689     0.921414      27.46
 O       4.709335    -1.537629    -0.280447     316.37
 H       5.428445    -1.985708    -0.811026      28.79
 C       6.479903     0.122004    -0.522182     114.37
 O       7.051684     1.463351    -0.526904     298.80
 H       7.357409     1.567639     0.401580      31.70
 H       6.703621    -0.279525    -1.553288      33.56
 H       6.988591    -0.501893     0.232119      32.06
55
name= lig-ACN-Water-frame_304
 C      -3.907583     0.750840    -2.874778      56.10
 H      -4.090809    -0.199466    -3.362356      20.59
 C      -3.894050     2.269265    -0.913555      41.43
 H      -4.106513     2.302848     0.270764      17.40
 C      -3.893771     3.387072    -1.836886      13.88
 O      -3.920270     4.760905    -1.444422     226.21
 C      -4.391194     4.876698    -0.072837     119.56
 H      -3.856997     4.318715     0.746523      23.39
 H      -5.493324     4.611738     0.085211      24.55
 H      -4.267015     5.953486     0.072433      24.74
 C      -3.873625     3.237038    -3.249312      17.60
 O      -3.949904     4.150487    -4.213699     137.64
 H      -3.964933     5.108104    -3.719379      20.15
 C      -3.900262     1.866697    -3.733882      28.96
 H      -3.831442     1.722469    -4.865395      23.49
 C      -3.970559     0.911654    -1.478664      20.30
 C      -3.796307    -0.284199    -0.552157      81.28
 H      -4.506011    -1.238932    -0.886510      21.87
 O      -4.365922    -0.208594     0.828076     205.45
 H      -3.655203     0.025518     1.457682      24.85
 C      -2.406038    -1.016806    -0.558863      87.83
 H      -1.979258    -1.050670    -1.576248      23.78
 C      -2.475569    -2.386145     0.151555     113.31
 O      -3.242081    -3.417866    -0.676637     163.57
 H      -2.854767    -3.355118    -1.664479      27.45
 H      -3.075090    -2.435990     1.069853      24.02
 H      -1.507424    -2.866288     0.227685      24.37
 C       1.767793    -0.557663    -1.359808      11.16
 H       2.306684    -1.024029    -2.200174      18.46
 C       2.033950     0.639925     0.798812      80.10
 H       2.685288     1.357699     1.515782      15.88
 C       0.589691     0.379680     1.053143       2.64
 O      -0.104776     0.868717     2.213827     238.18
 C      -0.052206     2.300695     2.363537     103.23
 H       0.144100     2.705465     3.519722      22.26
 H       0.648718     2.748807     1.703349      24.54
 H      -0.956541     2.883391     2.106734      23.43
 C      -0.238421    -0.066691     0.057193      12.31
 O      -1.649086    -0.080030     0.258274     178.34
 C       0.396252    -0.642225    -1.166565      82.29
 H      -0.160160    -1.491315    -1.884585      18.63
 C       2.606927     0.235888    -0.463316      22.64
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 C       4.011420     0.649173    -0.928453      83.11
 H       3.976454     0.524814    -1.968044      21.93
 O       4.061245     2.116868    -0.976890     239.13
 H       4.284565     2.528930    -0.103412      22.54
 C       5.070252    -0.118009    -0.100081     118.94
 H       4.970326     0.006755     0.949232      26.47
 O       4.763821    -1.493489    -0.309795     384.05
 H       5.401936    -1.871108    -0.943403      28.47
 C       6.553793     0.113763    -0.527871     114.15
 O       7.070875     1.447535    -0.442883     326.31
 H       7.116171     1.741320     0.536897      31.09
 H       6.568591    -0.185528    -1.631535      31.98
 H       7.229970    -0.546776    -0.015390      29.64
55
name= lig-ACN-Water-frame_305
 C      -3.882036     0.787784    -2.833812      52.68
 H      -4.109146    -0.279330    -3.154994      23.33
 C      -3.962139     2.316138    -0.995005      63.07
 H      -4.001348     2.381110     0.142034      21.42
 C      -3.908659     3.461769    -1.834468      16.76
 O      -3.979391     4.760222    -1.342479     205.28
 C      -4.383989     4.870645     0.022520      97.24
 H      -3.729744     4.186789     0.564175      26.30
 H      -5.514886     4.569306     0.058605      26.12
 H      -4.176024     5.910021     0.560573      24.18
 C      -3.991851     3.125643    -3.264721      17.95
 O      -3.880274     4.176341    -4.258710      67.01
 H      -4.217129     5.122193    -3.917491      21.50
 C      -3.928876     1.837737    -3.729548      68.43
 H      -4.081971     1.622939    -4.844953      21.55
 C      -3.891599     1.039809    -1.445081      26.61
 C      -3.816899    -0.255266    -0.580539      62.27
 H      -4.495671    -1.015144    -1.268958      22.54
 O      -4.367815    -0.128799     0.853538     209.72
 H      -3.621283     0.069750     1.503695      23.29
 C      -2.429804    -0.946935    -0.561297      85.84
 H      -2.126196    -1.030281    -1.576450      24.27
 C      -2.520221    -2.445243     0.134686     105.45
 O      -3.227383    -3.376491    -0.653057     253.60
 H      -2.718630    -3.518236    -1.509455      27.77
 H      -2.990036    -2.163616     1.097469      23.30
 H      -1.425430    -2.698521     0.502861      22.95
 C       1.818885    -0.513954    -1.317263      30.59
 H       2.150762    -0.878739    -2.250607      19.08
 C       1.963864     0.726301     0.727616      73.66
 H       2.616623     1.376867     1.560361      15.50
 C       0.649692     0.370831     1.031657      -6.66
 O      -0.046921     0.848756     2.202522     225.59
 C      -0.048133     2.340150     2.300140      85.94
 H       0.139553     2.490811     3.491370      21.69
 H       0.879126     2.708002     1.812295      22.14
 H      -1.051072     2.581245     1.953156      22.96
 C      -0.237055    -0.127099    -0.099028      15.07
 O      -1.564031    -0.119504     0.207442     199.92
 C       0.389389    -0.674516    -1.152649      68.61
 H      -0.216362    -1.189315    -2.041147      17.78
 C       2.552956     0.236631    -0.445190      32.11
 C       3.976305     0.654129    -0.947821      66.06
 H       4.193499     0.149401    -1.914176      21.82
 O       4.061600     2.113110    -0.997484     215.72
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 H       4.341215     2.431818    -0.053147      19.48
 C       5.197110    -0.095230    -0.106066      88.51
 H       5.058449     0.153587     0.931840      21.71
 O       4.838299    -1.538763    -0.329515     357.90
 H       5.123033    -1.848513    -1.241374      27.19
 C       6.636135     0.087502    -0.582661     107.72
 O       7.080401     1.477289    -0.353614     313.72
 H       7.049355     1.584192     0.682390      31.48
 H       6.673420    -0.026972    -1.714183      31.59
 H       7.230570    -0.625986    -0.144200      30.81
55
name= lig-ACN-Water-frame_306
 C      -3.930993     0.744546    -2.805653      47.07
 H      -3.642623    -0.317870    -3.205078      24.81
 C      -3.986064     2.390121    -0.957908      54.77
 H      -3.884839     2.684697     0.014303      24.92
 C      -4.016016     3.451718    -1.887766      16.87
 O      -4.022035     4.770511    -1.329006     164.22
 C      -4.364828     4.829510     0.187188      91.94
 H      -3.849045     4.227765     0.925480      25.66
 H      -5.536090     4.605593     0.372970      24.69
 H      -4.207492     6.060350     0.323879      22.96
 C      -4.010294     3.253846    -3.285146      14.57
 O      -3.845530     4.195824    -4.263571     159.51
 H      -4.305054     4.994276    -4.107262      27.32
 C      -4.000606     1.823977    -3.756242      16.96
 H      -4.106815     1.654738    -4.866122      19.62
 C      -3.791107     1.018848    -1.410963      -6.82
 C      -3.892345    -0.231712    -0.503842      81.59
 H      -4.777561    -0.951250    -0.894307      21.62
 O      -4.360357    -0.028959     0.751285     246.87
 H      -3.602616     0.062233     1.433358      23.86
 C      -2.524220    -0.998506    -0.562929      89.91
 H      -2.226266    -1.150890    -1.532714      27.33
 C      -2.533553    -2.304878     0.149489     118.36
 O      -3.177747    -3.334233    -0.668241     225.54
 H      -2.592863    -3.745734    -1.257247      31.66
 H      -3.208180    -2.451925     1.004840      24.03
 H      -1.435106    -2.778949     0.342100      23.42
 C       1.766454    -0.495105    -1.393196      40.12
 H       2.330088    -0.773499    -2.218440      24.52
 C       1.908942     0.746354     0.687728      82.86
 H       2.539171     1.242745     1.629260      19.88
 C       0.575977     0.489213     0.913616      32.86
 O       0.075473     0.814303     2.158359     240.32
 C      -0.047089     2.317015     2.291423      89.61
 H      -0.141458     2.630589     3.424677      23.29
 H       0.796844     2.926743     1.763737      23.00
 H      -0.898462     2.822287     1.759881      25.30
 C      -0.129597    -0.210157    -0.005979      21.36
 O      -1.495301    -0.132554     0.176217     158.98
 C       0.445435    -0.724383    -1.243815      64.68
 H      -0.191830    -1.037694    -2.074549      19.37
 C       2.613590     0.273138    -0.452554      49.25
 C       4.027308     0.621978    -0.877589      77.06
 H       3.993073     0.435674    -2.027453      23.70
 O       4.090700     2.078490    -1.065315     180.57
 H       4.272005     2.600825    -0.164133      21.46
 C       5.180536    -0.153353    -0.195504     105.93
 H       5.257543     0.012676     0.892847      21.30
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 O       4.912905    -1.559757    -0.306321     338.89
 H       5.171545    -1.825616    -1.253000      29.17
 C       6.688638     0.165213    -0.667817     116.66
 O       7.067572     1.476351    -0.283683     299.00
 H       7.402791     1.548191     0.651904      28.39
 H       6.890443     0.013706    -1.765373      33.20
 H       7.286257    -0.482287    -0.182043      32.26
55
name= lig-ACN-Water-frame_307
 C      -3.895495     0.827345    -2.826924      45.27
 H      -3.830690    -0.245113    -3.308048      21.29
 C      -3.936746     2.313503    -0.960802      54.93
 H      -4.001027     2.328391     0.023212      22.41
 C      -4.122405     3.480698    -1.853358      -0.92
 O      -4.087962     4.743192    -1.254615     163.46
 C      -4.366955     4.881693     0.207881      85.45
 H      -3.554305     4.437760     0.780968      24.85
 H      -5.529283     4.532999     0.419185      22.30
 H      -4.241517     6.152246     0.368488      21.91
 C      -4.015251     3.221384    -3.318699      19.52
 O      -3.842950     4.251040    -4.300232     150.85
 H      -4.043821     5.097804    -3.893825      22.53
 C      -4.074475     1.899089    -3.682539      69.86
 H      -3.895446     1.689132    -4.726646      27.24
 C      -3.865539     1.012840    -1.436128      33.68
 C      -3.861182    -0.211692    -0.543771      84.73
 H      -4.516817    -0.987292    -1.143333      25.49
 O      -4.396378     0.106842     0.816261     232.35
 H      -3.636930     0.251887     1.463243      24.16
 C      -2.526078    -0.986341    -0.541586      94.83
 H      -2.294938    -1.151448    -1.531223      29.54
 C      -2.572426    -2.348757     0.214322      97.52
 O      -3.165990    -3.344558    -0.722207     207.17
 H      -2.367794    -3.551230    -1.345089      27.56
 H      -2.963752    -2.079869     1.209252      25.25
 H      -1.371578    -2.495068     0.471357      23.78
 C       1.904152    -0.431947    -1.497785      39.01
 H       2.247478    -0.824530    -2.409948      18.44
 C       2.027768     0.729996     0.667679      31.71
 H       2.636421     1.340436     1.489251      16.84
 C       0.622267     0.553221     0.844647      -7.85
 O       0.124594     0.905021     2.143917     210.49
 C      -0.078267     2.322915     2.278837      95.22
 H      -0.273869     2.469162     3.371242      23.90
 H       1.004380     2.799334     2.070866      21.76
 H      -1.010623     2.484747     1.658006      23.86
 C      -0.194714    -0.307171    -0.075367      -3.95
 O      -1.574010    -0.159596     0.139109     158.39
 C       0.449707    -0.713056    -1.254907      61.98
 H      -0.020930    -1.361200    -1.888277      26.30
 C       2.593188     0.253084    -0.519458      28.55
 C       4.030896     0.625715    -0.936151      64.71
 H       4.149260     0.068945    -2.011698      22.25
 O       4.163373     2.078664    -1.109576     170.06
 H       4.243214     2.537230    -0.175216      22.09
 C       5.250016    -0.177824    -0.243839      80.68
 H       5.118306     0.079423     0.859083      23.01
 O       4.965625    -1.591345    -0.310122     346.02
 H       5.412042    -2.085669    -1.040404      28.81
 C       6.676870     0.186252    -0.691220     112.56
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 O       7.065673     1.532061    -0.290837     301.88
 H       7.062385     1.570654     0.694858      31.81
 H       6.715283     0.198372    -1.791131      31.89
 H       7.287881    -0.565569    -0.349385      32.95
55
name= lig-ACN-Water-frame_308
 C      -3.906479     0.844137    -2.892924      40.69
 H      -4.102470    -0.198999    -3.328266      21.22
 C      -3.968116     2.291121    -0.976758      69.73
 H      -4.073845     2.524243     0.017441      20.26
 C      -4.107006     3.426287    -1.748388      21.53
 O      -4.179607     4.726301    -1.250909     216.05
 C      -4.326407     4.959489     0.118825     102.71
 H      -3.545702     4.487425     0.788901      24.57
 H      -5.340968     4.343030     0.525759      22.79
 H      -4.544893     6.201396     0.382492      21.40
 C      -4.053175     3.324959    -3.180536      12.92
 O      -3.877878     4.283958    -4.260172     119.35
 H      -3.822181     5.295150    -3.899989      19.68
 C      -4.024281     1.987593    -3.754299      35.80
 H      -4.063578     1.836288    -4.791203      28.48
 C      -3.952731     0.992542    -1.495001      30.34
 C      -3.859930    -0.202922    -0.551004      80.98
 H      -4.684438    -0.942770    -0.781451      26.33
 O      -4.435868     0.199636     0.836443     202.20
 H      -3.720712     0.269757     1.513637      24.29
 C      -2.513014    -0.989367    -0.528289      92.73
 H      -2.186674    -1.150239    -1.510984      27.51
 C      -2.569675    -2.385875     0.203469     107.61
 O      -3.140179    -3.336316    -0.681228     211.48
 H      -2.682844    -3.473197    -1.612787      26.80
 H      -3.338682    -2.602066     0.953362      23.94
 H      -1.504738    -2.918828     0.532491      22.65
 C       1.802177    -0.447017    -1.543492      42.34
 H       2.345365    -0.732245    -2.445943      24.55
 C       2.060973     0.687799     0.585247      60.19
 H       2.670196     1.278093     1.313094      20.83
 C       0.689958     0.463626     0.853086      19.96
 O       0.136723     0.923224     2.069447     247.86
 C      -0.121819     2.356543     2.300192      99.62
 H      -0.548820     2.436390     3.288365      25.46
 H       0.787689     3.136388     2.177479      23.43
 H      -0.763026     2.931534     1.522311      24.66
 C      -0.161428    -0.146255    -0.121109       4.63
 O      -1.577280    -0.145443     0.147402     150.15
 C       0.514493    -0.761613    -1.264711      69.21
 H       0.078086    -1.405230    -1.847757      22.89
 C       2.708634     0.267985    -0.639609      24.65
 C       4.106267     0.574245    -1.081050      67.75
 H       4.294955     0.343663    -2.291805      20.73
 O       4.239487     2.045514    -1.134154     155.51
 H       4.318845     2.436152    -0.241607      25.61
 C       5.228773    -0.150757    -0.187171      94.48
 H       5.227019     0.124535     0.941844      23.58
 O       5.003244    -1.625651    -0.314421     306.44
 H       5.597985    -1.916594    -1.051078      27.93
 C       6.638463     0.225431    -0.740530     117.35
 O       7.013671     1.560118    -0.304004     278.27
 H       7.225326     1.683251     0.647605      30.32
 H       6.609711     0.294250    -1.807835      33.04
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 H       7.416610    -0.457224    -0.487966      31.93
55
name= lig-ACN-Water-frame_309
 C      -4.031797     0.864542    -3.007474      63.25
 H      -3.911465    -0.106041    -3.526329      26.76
 C      -4.071578     2.301299    -0.899393      47.60
 H      -3.922917     2.227539     0.210266      22.34
 C      -4.045100     3.471981    -1.784595      14.45
 O      -4.248557     4.761154    -1.339608     183.98
 C      -4.350943     4.951701     0.135876      86.64
 H      -3.319041     4.887978     0.655817      25.67
 H      -5.345445     4.381643     0.605083      23.79
 H      -4.556123     6.194011     0.050825      23.04
 C      -4.029642     3.342982    -3.199643      23.07
 O      -3.938412     4.335217    -4.097156     165.46
 H      -4.243916     5.317209    -3.783192      20.78
 C      -3.954800     2.065234    -3.758880      44.54
 H      -4.093810     2.143490    -4.795763      21.15
 C      -3.962648     0.968605    -1.520576     -24.55
 C      -3.999980    -0.214145    -0.447477      81.17
 H      -4.610796    -1.029633    -0.907700      24.85
 O      -4.435031     0.235035     0.768411     238.78
 H      -3.692231     0.287929     1.424102      23.79
 C      -2.483506    -1.040579    -0.466517      57.14
 H      -2.290708    -1.144423    -1.522829      25.73
 C      -2.604674    -2.451148     0.169641     112.68
 O      -3.201631    -3.419668    -0.736386     249.76
 H      -2.735275    -3.392109    -1.562201      29.21
 H      -3.172729    -2.178293     1.069490      25.46
 H      -1.485205    -2.585841     0.636785      23.43
 C       1.855409    -0.471970    -1.585279      47.65
 H       2.112781    -0.989129    -2.544757      23.03
 C       2.117620     0.646982     0.486192      53.16
 H       2.678743     1.084103     1.245402      20.27
 C       0.761080     0.463268     0.821798      13.63
 O       0.128895     0.928678     1.997463     215.06
 C      -0.151842     2.469796     2.282818      80.05
 H      -0.743221     2.396797     3.154162      25.94
 H       0.918887     2.808073     2.554943      22.82
 H      -0.852516     2.717272     1.393176      23.23
 C      -0.118386    -0.061186    -0.163252      11.13
 O      -1.434093    -0.064511     0.196019     109.80
 C       0.426027    -0.778883    -1.235389      62.76
 H      -0.178617    -1.201139    -1.911915      21.17
 C       2.674552     0.247935    -0.771529      27.28
 C       4.192702     0.583102    -1.116761      64.19
 H       4.327158     0.077846    -2.290051      20.96
 O       4.315753     2.012814    -1.160441     212.63
 H       4.340171     2.354936    -0.266162      27.57
 C       5.203153    -0.178750    -0.239885      91.04
 H       4.973235     0.100577     0.885330      23.23
 O       5.048848    -1.568980    -0.295745     339.56
 H       5.267116    -1.935701    -1.224112      27.65
 C       6.614064     0.299590    -0.766614     110.67
 O       6.945419     1.621989    -0.296432     270.40
 H       7.426823     1.439219     0.563509      28.73
 H       6.571836     0.288799    -1.812169      36.59
 H       7.344670    -0.467900    -0.438495      32.01
55
name= lig-ACN-Water-frame_310
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 C      -4.068981     0.906229    -2.948614      70.15
 H      -4.018908    -0.013562    -3.467149      29.59
 C      -4.088135     2.273123    -1.009680      58.37
 H      -4.170162     2.544194     0.149707      22.85
 C      -4.058858     3.434793    -1.743822      -3.67
 O      -4.299998     4.803929    -1.364835     159.23
 C      -4.372859     5.056000     0.048447     108.40
 H      -3.337057     4.701065     0.541687      25.08
 H      -5.055609     4.226154     0.579583      23.23
 H      -4.756944     6.126291     0.403326      23.20
 C      -3.959186     3.307973    -3.168723      10.01
 O      -4.021258     4.486759    -3.972448     113.09
 H      -4.461605     5.175046    -3.527764      20.39
 C      -3.967199     2.058393    -3.780337      55.03
 H      -3.721310     1.843270    -4.814876      27.03
 C      -4.036191     1.003096    -1.561195      22.30
 C      -3.912437    -0.262815    -0.579596      54.23
 H      -4.664134    -0.999380    -0.847228      24.84
 O      -4.464636     0.213242     0.764040     166.55
 H      -3.692760     0.356279     1.414395      24.16
 C      -2.542854    -0.912881    -0.451974      80.56
 H      -2.143665    -1.034253    -1.502546      26.44
 C      -2.581633    -2.389957     0.202748      99.49
 O      -3.275548    -3.459191    -0.746786     177.88
 H      -2.667208    -3.738888    -1.446158      29.12
 H      -3.230718    -2.602199     1.063785      25.66
 H      -1.631351    -3.033639     0.295816      24.16
 C       1.770316    -0.616499    -1.674634      41.93
 H       2.226596    -0.997861    -2.636301      20.46
 C       2.196821     0.663246     0.473288      41.29
 H       2.855592     1.035384     1.105118      22.49
 C       0.786061     0.617208     0.755087      -6.17
 O       0.134640     0.962051     1.983836     216.36
 C      -0.137503     2.372211     2.228797     113.73
 H      -0.863875     2.484988     2.993349      26.47
 H       0.718045     3.064130     2.511286      25.97
 H      -0.367552     3.077035     1.311370      26.09
 C      -0.073058    -0.141995    -0.132187      -5.58
 O      -1.458622    -0.069057     0.206592      99.93
 C       0.451580    -0.689750    -1.324655      73.52
 H      -0.218959    -1.274351    -1.948704      26.44
 C       2.661412     0.194273    -0.841282      16.28
 C       4.066774     0.531274    -1.135597      75.17
 H       4.427317     0.272668    -2.342672      23.39
 O       4.369271     1.995825    -1.185561     133.17
 H       4.539489     2.410939    -0.259604      23.78
 C       5.216188    -0.114756    -0.323100      81.65
 H       5.169266     0.223603     0.816789      23.58
 O       5.054596    -1.560127    -0.300436     295.68
 H       5.138015    -1.935766    -1.253143      28.67
 C       6.590005     0.316176    -0.741987     100.45
 O       6.923187     1.683762    -0.282045     234.68
 H       7.158442     1.840889     0.717106      26.24
 H       6.691656     0.398015    -1.778981      31.60
 H       7.366927    -0.453190    -0.384286      30.14
55
name= lig-ACN-Water-frame_311
 C      -4.026828     0.868860    -2.934912      62.07
 H      -4.170175    -0.090002    -3.293872      21.29
 C      -4.091570     2.334895    -0.978460      44.69
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 H      -4.335741     2.230752     0.214845      17.85
 C      -4.145432     3.484547    -1.819135      15.06
 O      -4.344504     4.806545    -1.387921     203.55
 C      -4.367304     5.022237     0.033077     107.99
 H      -3.277291     5.055399     0.579819      24.62
 H      -5.172451     4.342716     0.473052      23.83
 H      -4.727575     6.065835     0.103618      25.12
 C      -3.964499     3.399957    -3.204027       0.85
 O      -4.084754     4.520531    -3.878071     125.86
 H      -4.102302     5.349541    -3.371513      20.05
 C      -3.948092     2.024723    -3.784780      31.77
 H      -3.811295     1.968130    -4.912673      23.65
 C      -4.089101     0.985791    -1.528376      17.69
 C      -3.891504    -0.160669    -0.612027      83.35
 H      -4.355505    -1.024737    -1.070722      27.88
 O      -4.477072     0.108737     0.699132     190.49
 H      -3.725127     0.278834     1.378199      23.02
 C      -2.475633    -0.918606    -0.501151      69.47
 H      -2.199025    -1.169545    -1.613660      27.78
 C      -2.611266    -2.470322     0.113660     102.16
 O      -3.346420    -3.378767    -0.704414     221.69
 H      -2.710210    -3.844450    -1.408263      26.45
 H      -3.049018    -2.380929     1.117035      26.88
 H      -1.492904    -2.500398     0.303410      27.11
 C       1.815923    -0.604520    -1.699433      35.95
 H       2.148776    -1.024922    -2.681354      19.12
 C       2.148658     0.698158     0.403490      50.49
 H       2.811458     1.202771     0.984193      20.54
 C       0.774426     0.656510     0.710850       5.45
 O       0.201439     1.000731     1.955915     236.10
 C      -0.067237     2.405487     2.152879     103.02
 H      -1.017878     2.442569     2.743361      24.87
 H       0.780751     2.737472     2.709742      24.17
 H      -0.401454     2.754219     1.118057      25.58
 C      -0.091444    -0.156143    -0.112470     -20.07
 O      -1.521619    -0.109037     0.204093     106.66
 C       0.398743    -0.711329    -1.394451      50.29
 H      -0.239382    -1.420279    -2.075292      24.36
 C       2.608847     0.103194    -0.802040      19.15
 C       4.090435     0.553019    -1.228317      62.16
 H       4.010096     0.164261    -2.467104      22.34
 O       4.316322     1.982997    -1.215670     154.73
 H       4.762959     2.224056    -0.333025      20.25
 C       5.165957    -0.104015    -0.321049      83.82
 H       4.981915     0.204225     0.819267      22.86
 O       5.035878    -1.554526    -0.310902     305.97
 H       5.520413    -1.864736    -1.148622      27.86
 C       6.662051     0.402309    -0.726258      90.40
 O       6.926508     1.745680    -0.270060     285.11
 H       7.018544     1.685888     0.714436      30.66
 H       6.783027     0.351323    -1.786300      30.94
 H       7.396930    -0.364966    -0.199906      29.84
55
name= lig-ACN-Water-frame_312
 C      -3.997492     0.889849    -2.968545      62.26
 H      -3.923768    -0.013977    -3.500029      27.58
 C      -4.163917     2.369838    -0.942345      80.58
 H      -4.085588     2.620342     0.217929      23.22
 C      -4.213719     3.456599    -1.775921      20.42
 O      -4.363785     4.773937    -1.406640     194.09
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 C      -4.419838     5.059988     0.036363     112.22
 H      -3.292671     4.809566     0.474348      26.21
 H      -5.054734     4.477605     0.640193      27.76
 H      -4.677564     6.022826     0.160436      27.06
 C      -4.048872     3.305272    -3.190211      16.18
 O      -4.117014     4.530826    -3.969737     122.17
 H      -3.832294     5.363631    -3.354380      19.37
 C      -3.918545     2.075966    -3.746626      33.24
 H      -4.111374     1.976579    -4.879140      17.91
 C      -4.011105     1.114893    -1.522346       6.37
 C      -3.880086    -0.213684    -0.624449      71.13
 H      -4.597014    -0.873828    -1.071709      23.78
 O      -4.496106    -0.039213     0.641654     183.30
 H      -3.826252     0.168786     1.352890      25.41
 C      -2.494832    -0.994796    -0.614168      82.21
 H      -2.070969    -0.926144    -1.725907      24.62
 C      -2.553994    -2.354842     0.061567     121.64
 O      -3.392214    -3.282649    -0.663645     207.45
 H      -2.901802    -3.552609    -1.519604      26.96
 H      -3.060872    -2.273409     1.042995      25.85
 H      -1.647489    -3.013601     0.156011      23.94
 C       1.746270    -0.549432    -1.644898      46.70
 H       2.162975    -0.982137    -2.555184      25.76
 C       2.055473     0.742414     0.321766      43.14
 H       2.554827     1.457492     1.013927      20.90
 C       0.688973     0.500673     0.676707      12.75
 O       0.291371     0.978922     1.916631     229.35
 C      -0.030598     2.479156     2.072329      98.21
 H      -0.974379     2.565218     2.743022      25.12
 H       0.711863     3.064325     2.518676      26.69
 H      -0.060310     3.071635     1.116748      27.17
 C      -0.173951    -0.144868    -0.250464      25.18
 O      -1.478999    -0.177852     0.183080     129.46
 C       0.400173    -0.783803    -1.305985      70.61
 H      -0.365952    -1.303378    -2.110135      21.24
 C       2.682104     0.142656    -0.813937      27.33
 C       4.061550     0.511836    -1.263006      78.49
 H       4.501432     0.140420    -2.433848      22.47
 O       4.200149     1.973383    -1.261854     176.08
 H       4.854034     2.236427    -0.615583      23.35
 C       5.174053    -0.110486    -0.365805      92.11
 H       4.814305     0.263292     0.682244      23.90
 O       5.062044    -1.522830    -0.308747     318.17
 H       5.317757    -1.989310    -1.169339      27.98
 C       6.641687     0.417213    -0.651434      91.46
 O       6.931096     1.801417    -0.254656     275.59
 H       7.373738     1.888499     0.603087      27.96
 H       6.856561     0.378080    -1.736553      31.08
 H       7.435096    -0.305058    -0.130896      29.33
55
name= lig-ACN-Water-frame_313
 C      -3.913895     1.002555    -2.897613      72.91
 H      -3.771625    -0.026431    -3.253080      31.79
 C      -4.173745     2.340389    -0.903176      37.97
 H      -4.099605     2.453322     0.205642      34.66
 C      -4.264542     3.489564    -1.777919      13.15
 O      -4.415887     4.794722    -1.361007     196.74
 C      -4.418423     5.078478     0.048952     113.71
 H      -3.359061     4.740055     0.576607      26.97
 H      -5.193700     4.529580     0.394956      27.08
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 H      -4.521300     6.055993     0.202587      27.66
 C      -4.155574     3.402082    -3.195591      10.33
 O      -4.119090     4.404481    -4.077681     106.17
 H      -4.227783     5.332834    -3.660882      21.15
 C      -3.992210     2.089812    -3.797665      22.98
 H      -3.789729     1.959649    -4.932066      22.33
 C      -3.885436     1.045545    -1.516074     -17.57
 C      -3.904831    -0.274302    -0.752464      54.75
 H      -4.436325    -1.000589    -1.281851      24.38
 O      -4.506234    -0.170785     0.666764      95.27
 H      -3.865580     0.160893     1.314527      27.91
 C      -2.486790    -0.938683    -0.698289      82.73
 H      -2.153960    -1.168752    -1.840104      27.22
 C      -2.506411    -2.331266     0.019392     114.38
 O      -3.461476    -3.189295    -0.680698     220.34
 H      -3.176761    -3.458208    -1.523565      29.89
 H      -2.948754    -2.109744     1.006009      26.81
 H      -1.411591    -2.582228     0.168981      26.73
 C       1.754735    -0.591439    -1.629598      56.91
 H       2.086956    -0.997266    -2.561603      27.73
 C       1.998258     0.771341     0.272299      37.13
 H       2.642484     1.456141     1.025973      23.03
 C       0.728993     0.466093     0.647766      22.13
 O       0.301931     1.028824     1.907725     214.30
 C       0.060056     2.526522     1.965581     107.59
 H      -0.989679     2.619953     2.541112      26.55
 H       0.874331     2.871250     2.498630      28.83
 H      -0.162393     2.814550     0.956371      28.84
 C      -0.216329    -0.162337    -0.228382      13.79
 O      -1.547847    -0.259552     0.133941     130.89
 C       0.411233    -0.830049    -1.328636      48.65
 H      -0.122779    -1.563432    -2.188189      23.37
 C       2.611094     0.240108    -0.884356      18.36
 C       4.112883     0.506690    -1.265673      79.46
 H       4.080338     0.040633    -2.501438      22.79
 O       4.094761     1.982195    -1.335004     146.85
 H       4.771564     2.309319    -0.702229      21.58
 C       5.181757    -0.040380    -0.308777      96.45
 H       5.076803     0.233930     0.791144      22.78
 O       5.112675    -1.525784    -0.295248     289.29
 H       5.170016    -1.724049    -1.278469      28.08
 C       6.619913     0.409510    -0.593779      90.67
 O       6.932059     1.847768    -0.268162     249.82
 H       7.132408     1.790626     0.712029      26.59
 H       6.878286     0.298881    -1.701815      29.05
 H       7.264225    -0.346806     0.046800      29.14
55
name= lig-ACN-Water-frame_314
 C      -3.782509     1.003505    -2.908638       9.15
 H      -3.674031     0.043586    -3.518112      18.61
 C      -4.110198     2.319148    -0.921728      68.88
 H      -4.403570     2.328478     0.069214      21.93
 C      -4.306571     3.498574    -1.775227      -0.12
 O      -4.456456     4.859913    -1.335594     164.16
 C      -4.447764     5.051595     0.112141     119.94
 H      -3.512719     4.567398     0.661986      26.27
 H      -5.277469     4.823251     0.622707      28.24
 H      -4.364464     6.116782     0.190961      26.00
 C      -4.245270     3.350671    -3.226457      11.79
 O      -4.133339     4.381160    -4.221944     137.64
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 H      -4.565443     5.162161    -4.032465      22.45
 C      -4.043671     2.102446    -3.735779      57.68
 H      -3.727306     2.071655    -4.811333      30.36
 C      -3.910299     1.059190    -1.461072      22.03
 C      -3.879820    -0.304302    -0.735558     112.28
 H      -4.520998    -0.910852    -1.254645      30.05
 O      -4.463328    -0.273423     0.571610     186.17
 H      -3.751907    -0.035576     1.219840      26.44
 C      -2.512529    -0.984872    -0.733649      94.21
 H      -2.046195    -0.962490    -1.837231      27.76
 C      -2.534986    -2.301341    -0.066088     128.20
 O      -3.463610    -3.119460    -0.702467     205.11
 H      -2.954165    -3.588071    -1.424268      29.02
 H      -2.766586    -2.258545     1.042446      27.46
 H      -1.589917    -2.863505    -0.170622      27.27
 C       1.810092    -0.661720    -1.710179      34.04
 H       2.261871    -1.206550    -2.507585      19.58
 C       2.053259     0.798288     0.257682      28.23
 H       2.857126     1.403084     1.014071      19.47
 C       0.679593     0.582977     0.672760      -0.64
 O       0.238595     1.052366     1.873291     250.96
 C       0.126304     2.487088     1.832695     113.56
 H      -0.751006     2.825559     2.558150      25.37
 H       0.957388     3.028958     2.187056      27.37
 H       0.033001     2.881006     0.849206      29.95
 C      -0.153067    -0.275978    -0.190298     -20.81
 O      -1.586402    -0.215146     0.095090     125.84
 C       0.401127    -0.846610    -1.368456      60.38
 H      -0.294761    -1.698937    -1.897519      22.57
 C       2.548430     0.245487    -0.933315      32.17
 C       3.970514     0.588823    -1.227249      80.46
 H       4.514169     0.035582    -2.289442      23.28
 O       4.069912     2.022442    -1.442355     161.12
 H       4.579688     2.440749    -0.640655      23.11
 C       5.160813    -0.034625    -0.214700      74.67
 H       4.741308     0.274876     0.755904      26.62
 O       5.153480    -1.458264    -0.300874     287.76
 H       5.567744    -1.849425    -1.119427      30.20
 C       6.646745     0.444022    -0.567786      94.82
 O       6.900992     1.804710    -0.290440     298.23
 H       7.095530     1.927378     0.719138      25.97
 H       6.914495     0.134214    -1.678275      30.75
 H       7.357202    -0.169782     0.110151      29.85
55
name= lig-ACN-Water-frame_315
 C      -3.720469     0.913887    -2.924402      76.89
 H      -3.368160    -0.115716    -3.358317      25.72
 C      -4.162019     2.403948    -0.959527      82.73
 H      -4.260919     2.577477     0.007300      24.27
 C      -4.328136     3.545646    -1.793631      10.01
 O      -4.494503     4.809263    -1.297048     173.35
 C      -4.474994     5.084285     0.185363     110.57
 H      -3.715145     4.358337     0.607931      26.43
 H      -5.405127     4.827494     0.525236      27.42
 H      -4.137517     6.137654     0.460086      24.52
 C      -4.293091     3.393480    -3.219300      11.62
 O      -4.193866     4.352170    -4.312744      45.23
 H      -4.404313     5.316459    -3.993065      22.55
 C      -3.987228     2.068990    -3.701786       1.66
 H      -4.118415     1.920277    -4.757394      18.30
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 C      -3.919260     1.064664    -1.563629       6.46
 C      -3.884899    -0.287197    -0.759291      89.59
 H      -4.443492    -0.928753    -1.347292      28.65
 O      -4.381400    -0.309629     0.545250     194.67
 H      -3.737157    -0.047231     1.294197      23.66
 C      -2.440358    -0.947080    -0.752224      72.04
 H      -2.166140    -1.043614    -1.883874      28.65
 C      -2.462859    -2.405696    -0.112100     116.15
 O      -3.511082    -3.165326    -0.814018     191.52
 H      -3.049730    -3.842974    -1.492429      26.28
 H      -2.802402    -2.185608     0.956716      27.08
 H      -1.464462    -2.827311    -0.159827      27.20
 C       1.750543    -0.713243    -1.732569      42.39
 H       2.217833    -1.237441    -2.563814      24.03
 C       1.993710     0.767771     0.244255      45.48
 H       2.679906     1.536964     0.991851      19.71
 C       0.711396     0.565101     0.586980      13.21
 O       0.117334     1.073123     1.837744     228.05
 C       0.185086     2.579608     1.739095     102.48
 H      -0.655381     2.964004     2.427223      25.04
 H       1.188719     2.841694     2.023103      25.34
 H      -0.139412     2.845427     0.760569      29.22
 C      -0.127418    -0.264050    -0.176862       2.94
 O      -1.477027    -0.102853     0.060018     135.11
 C       0.447493    -0.916407    -1.321828      67.85
 H      -0.185551    -1.580016    -2.020348      23.69
 C       2.559276     0.191988    -0.925485      20.35
 C       4.028881     0.604624    -1.228597      58.67
 H       4.146460     0.153792    -2.477345      18.84
 O       4.087835     2.102361    -1.523374     193.90
 H       4.320370     2.569773    -0.680125      25.47
 C       5.093114     0.023075    -0.212397     110.49
 H       5.043982     0.179595     0.842980      26.56
 O       5.168266    -1.424430    -0.272604     271.24
 H       5.512001    -1.558962    -1.209668      27.31
 C       6.588040     0.415697    -0.475790      95.47
 O       6.876230     1.832691    -0.344031     271.94
 H       7.383372     1.868581     0.551658      26.59
 H       6.732058     0.279216    -1.653232      30.72
 H       7.267936    -0.276247     0.088631      30.64
55
name= lig-ACN-Water-frame_316
 C      -3.739379     0.949048    -2.929989      53.68
 H      -3.483541    -0.083802    -3.421600      23.24
 C      -4.237951     2.366711    -1.052869      79.18
 H      -4.079501     2.351428    -0.054793      27.11
 C      -4.328135     3.569949    -1.841746       7.84
 O      -4.521669     4.849799    -1.233907     173.20
 C      -4.503830     4.983367     0.204189     119.87
 H      -3.905488     4.395997     0.828046      28.99
 H      -5.502260     5.062724     0.560437      26.10
 H      -4.199282     6.152543     0.220768      23.36
 C      -4.212604     3.375070    -3.302630      17.32
 O      -4.315790     4.318556    -4.280849      74.83
 H      -4.124864     5.327633    -3.951056      21.40
 C      -3.955937     2.043732    -3.779163      64.03
 H      -3.917046     1.965807    -4.822371      24.29
 C      -3.898135     1.096125    -1.523645      -0.76
 C      -3.765904    -0.252136    -0.807042      75.15
 H      -4.357074    -0.990889    -1.280922      24.38
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 O      -4.352041    -0.294942     0.617545     160.75
 H      -3.672539     0.218150     1.150070      25.56
 C      -2.345441    -0.908246    -0.766511      88.44
 H      -1.874543    -0.994778    -1.779282      25.34
 C      -2.438140    -2.461131    -0.176207     107.81
 O      -3.483945    -3.233831    -0.931736     234.42
 H      -3.068640    -3.758482    -1.693920      26.56
 H      -2.816471    -2.512278     0.914231      24.81
 H      -1.471665    -2.923614    -0.210170      25.57
 C       1.811167    -0.683196    -1.631777      41.24
 H       2.041425    -1.059980    -2.649871      24.24
 C       2.000059     0.740353     0.210916      29.78
 H       2.678239     1.580340     0.859351      19.68
 C       0.656734     0.482000     0.669802      22.31
 O       0.023046     1.128894     1.698866     231.47
 C       0.186219     2.635228     1.679997      96.41
 H      -0.324569     3.061240     2.556650      25.64
 H       1.288037     2.917102     1.801961      24.93
 H      -0.090496     3.044074     0.713115      27.21
 C      -0.127312    -0.211286    -0.281137       5.26
 O      -1.451901    -0.066792    -0.027816     161.54
 C       0.439427    -1.014957    -1.290641      69.39
 H      -0.168286    -1.530541    -1.969552      23.32
 C       2.634175     0.151743    -0.901384      35.13
 C       4.042964     0.635614    -1.279089      57.02
 H       4.510030     0.077208    -2.398986      21.12
 O       4.102514     2.122082    -1.539646     211.43
 H       4.426838     2.542321    -0.753543      25.31
 C       5.099335     0.090978    -0.202741      91.65
 H       4.601293     0.434051     0.646177      25.03
 O       5.123451    -1.413065    -0.285101     287.03
 H       5.194876    -1.804033    -1.197346      26.71
 C       6.504063     0.453388    -0.533673      98.59
 O       6.901013     1.872213    -0.385827     275.81
 H       7.071765     1.961693     0.601974      28.31
 H       6.808835    -0.007630    -1.593358      28.04
 H       7.094093    -0.131194     0.176023      28.21
55
name= lig-ACN-Water-frame_317
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55
name= lig-ACN-Water-frame_318
 C      -3.820835     0.930686    -3.042836      55.65
 H      -3.592536    -0.032092    -3.497691      27.51
 C      -4.206529     2.324193    -1.010661      73.93
 H      -4.579846     2.079393     0.069486      24.46
 C      -4.300084     3.464620    -1.830175      17.25
 O      -4.522594     4.738624    -1.369544     181.16
 C      -4.588118     4.874091     0.152823     102.82
 H      -3.940828     4.296495     0.652078      29.25
 H      -5.735696     4.775402     0.377176      23.85
 H      -4.400331     6.000185     0.367405      24.20
 C      -4.163934     3.428494    -3.308240       4.78
 O      -4.507459     4.402083    -4.178037     171.11
 H      -4.696478     5.226152    -3.800632      25.05
 C      -3.802518     2.124642    -3.866838      12.33
 H      -3.824946     2.139334    -4.962960      19.92
 C      -3.872864     1.048715    -1.589715      -5.08
 C      -3.809664    -0.285937    -0.781416      92.92
 H      -4.493732    -1.072233    -1.231105      24.62
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 O      -4.325557    -0.144674     0.588888     217.40
 H      -3.549896     0.012803     1.146475      27.41
 C      -2.459845    -1.016351    -0.909296      82.10
 H      -2.149327    -1.067051    -1.912157      28.67
 C      -2.368144    -2.439951    -0.335394     112.77
 O      -3.431886    -3.184307    -1.060073     260.97
 H      -3.069729    -3.874013    -1.632316      27.43
 H      -2.717322    -2.485936     0.754033      26.15
 H      -1.303401    -2.755926    -0.266087      25.91
 C       1.949145    -0.749675    -1.609417      44.82
 H       2.388106    -1.484069    -2.320411      21.39
 C       2.104689     0.747787     0.357527      47.88
 H       2.727306     1.400386     1.027126      18.97
 C       0.672772     0.629436     0.510282       7.91
 O      -0.082488     1.255375     1.458060     204.45
 C       0.198001     2.706296     1.663940      92.95
 H      -0.174261     2.996645     2.600436      26.09
 H       1.427716     2.848931     1.691080      22.42
 H      -0.106490     3.269635     0.710187      26.22
 C      -0.074471    -0.305134    -0.260556       2.68
 O      -1.458268    -0.164161    -0.124522     120.36
 C       0.583374    -0.990737    -1.364352      64.84
 H       0.046545    -1.667398    -1.848328      25.27
 C       2.610037     0.235938    -0.875476      29.80
 C       3.967144     0.618222    -1.331704      66.55
 H       4.071682     0.001874    -2.517849      22.86
 O       4.124150     2.076445    -1.446491     153.30
 H       5.106615     2.257300    -1.181953      22.69
 C       5.156689     0.108704    -0.337129      86.30
 H       4.720130     0.621595     0.460447      28.19
 O       4.893285    -1.317346    -0.309197     297.50
 H       5.369770    -1.805938    -1.025677      30.42
 C       6.598999     0.490805    -0.619369     103.41
 O       6.836889     1.987016    -0.464117     262.72
 H       7.241539     2.075956     0.456433      27.77
 H       6.903729     0.231558    -1.705224      29.66
 H       7.218250    -0.096328     0.031067      30.63
55
name= lig-ACN-Water-frame_319
 C      -3.720860     0.976391    -3.073658      75.38
 H      -3.595822     0.079398    -3.571638      28.62
 C      -4.185982     2.198642    -1.055739      50.41
 H      -4.103247     2.451738     0.123546      21.20
 C      -4.256240     3.438767    -1.843540       6.61
 O      -4.530670     4.701998    -1.363733     202.17
 C      -4.643667     4.819385    -0.007034     116.50
 H      -3.960143     4.288468     0.547506      27.95
 H      -5.696859     4.449228     0.488992      24.05
 H      -4.459231     5.889815     0.137228      24.80
 C      -4.200273     3.339190    -3.235575      21.57
 O      -4.580436     4.428510    -4.117127     162.59
 H      -4.221858     5.372184    -3.919311      21.91
 C      -3.813520     2.156316    -3.789431      61.02
 H      -3.839616     1.986276    -4.905857      19.66
 C      -3.944239     0.995498    -1.700729      24.83
 C      -3.948402    -0.295631    -0.902740      37.87
 H      -4.809506    -0.977897    -1.321688      23.14
 O      -4.358021    -0.086909     0.556506     164.09
 H      -3.696712     0.220079     1.241193      23.73
 C      -2.422508    -0.969008    -0.942812      81.56
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 H      -2.180294    -0.964356    -1.936827      29.19
 C      -2.401241    -2.406427    -0.332334     113.98
 O      -3.466399    -3.157858    -1.056397     219.77
 H      -2.920750    -3.778492    -1.675524      26.24
 H      -2.592917    -2.361028     0.786365      25.28
 H      -1.521166    -2.985404    -0.755709      22.66
 C       1.965467    -0.757665    -1.566582      40.70
 H       2.547396    -1.090589    -2.434854      19.30
 C       2.039160     0.793137     0.294046      52.01
 H       2.601743     1.415508     0.882902      18.45
 C       0.650318     0.678481     0.446203       7.12
 O      -0.112242     1.325537     1.424512     216.79
 C       0.227383     2.727725     1.663944      98.28
 H      -0.387819     3.011816     2.518841      24.08
 H       1.455282     2.868965     1.899395      20.45
 H      -0.259148     3.426906     0.842429      24.40
 C      -0.038149    -0.292125    -0.381024      12.11
 O      -1.436909    -0.285979    -0.158987     167.86
 C       0.586191    -1.036411    -1.324845      74.12
 H       0.121210    -1.690369    -2.035646      23.76
 C       2.660260     0.218360    -0.827996      29.51
 C       4.069069     0.631184    -1.322468      67.02
 H       4.331139     0.201413    -2.555067      21.17
 O       4.148367     2.101722    -1.439853     164.41
 H       4.994755     2.350758    -1.020535      21.22
 C       5.102857     0.137560    -0.402175     100.09
 H       5.167518     0.356679     0.645314      22.84
 O       4.861535    -1.332060    -0.313331     314.71
 H       5.159976    -1.572303    -1.241327      28.94
 C       6.639378     0.510868    -0.743759      98.37
 O       6.793232     1.984719    -0.499598     246.97
 H       6.999391     2.045155     0.512363      26.95
 H       6.919874     0.253310    -1.783161      32.22
 H       7.336371     0.063098    -0.047768      32.31
55
name= lig-ACN-Water-frame_320
 C      -3.641121     0.944406    -3.097812      30.76
 H      -3.468333     0.092736    -3.653123      20.88
 C      -4.112085     2.237152    -1.116660      61.92
 H      -4.098588     2.171882     0.100527      19.58
 C      -4.275007     3.370254    -1.854920      25.34
 O      -4.525085     4.643453    -1.432139     221.42
 C      -4.686579     4.838621     0.045752     109.42
 H      -3.798544     4.444801     0.497372      27.22
 H      -5.735833     4.249378     0.293533      24.25
 H      -4.746471     5.796054     0.352343      26.36
 C      -4.220378     3.379160    -3.254612      20.50
 O      -4.626416     4.331262    -4.037145     219.79
 H      -4.278554     5.367702    -3.994208      17.08
 C      -3.876240     2.137535    -3.882217      22.35
 H      -3.486957     2.223189    -4.972994      24.56
 C      -4.004007     0.946061    -1.722527      33.82
 C      -3.898952    -0.273703    -0.813921     107.71
 H      -4.432435    -1.216619    -1.325198      25.54
 O      -4.441786    -0.064027     0.433937     239.94
 H      -3.588042     0.141698     0.972975      24.85
 C      -2.428096    -1.012472    -0.982551      86.57
 H      -2.128090    -0.997187    -1.952680      28.55
 C      -2.498287    -2.418199    -0.472906     121.59
 O      -3.545064    -3.158221    -1.008210     269.90
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 H      -3.223748    -3.826822    -1.755049      25.74
 H      -2.613596    -2.395179     0.646599      27.02
 H      -1.360655    -2.802050    -0.402380      24.22
 C       1.994307    -0.744823    -1.607064      43.40
 H       2.322204    -1.136168    -2.556145      24.62
 C       1.985633     0.917647     0.199444      62.15
 H       2.388002     1.614289     0.738964      23.17
 C       0.612537     0.647884     0.408694      10.93
 O      -0.126086     1.379199     1.386689     208.02
 C       0.180812     2.753078     1.709795      81.17
 H      -0.442381     3.026579     2.632622      24.50
 H       1.407841     2.940967     2.075525      21.02
 H       0.114297     3.402097     0.702636      24.44
 C      -0.147150    -0.210092    -0.464684      -3.12
 O      -1.455520    -0.306502    -0.139341     162.56
 C       0.663985    -1.095742    -1.356239      56.85
 H       0.049647    -1.813509    -2.051388      22.64
 C       2.740812     0.191176    -0.827534      16.99
 C       4.113957     0.755624    -1.269130      61.14
 H       4.306062     0.165391    -2.436581      22.46
 O       4.195884     2.158705    -1.459493     208.26
 H       4.547855     2.496583    -0.621804      22.98
 C       5.210548     0.038830    -0.347269      88.30
 H       4.868938     0.507731     0.610144      23.79
 O       4.908925    -1.339172    -0.359040     335.97
 H       5.095552    -1.822575    -1.221105      27.66
 C       6.622892     0.544644    -0.824100     100.20
 O       6.762904     1.943174    -0.566612     268.45
 H       6.979074     2.060222     0.415412      28.93
 H       6.826401     0.489786    -1.870626      31.21
 H       7.312681    -0.164908    -0.322648      29.75
55
name= lig-ACN-Water-frame_321
 C      -3.699052     0.922508    -3.184637      79.05
 H      -3.263836    -0.003696    -3.507160      25.63
 C      -4.083118     2.184176    -1.087918      37.34
 H      -4.432874     2.208996     0.024044      18.55
 C      -4.306936     3.388034    -1.882300       0.34
 O      -4.530702     4.696614    -1.389952     181.34
 C      -4.704112     4.793063     0.066343     112.67
 H      -3.873894     4.525552     0.776074      25.07
 H      -5.620922     4.111831     0.506015      24.01
 H      -4.988637     5.758218     0.024005      24.37
 C      -4.197612     3.237584    -3.317005       6.23
 O      -4.709733     4.335132    -4.108201     123.63
 H      -4.743786     5.180647    -3.480785      20.17
 C      -3.815439     2.068973    -3.947920      88.47
 H      -3.607885     2.150059    -5.073967      22.73
 C      -3.895836     0.957909    -1.758400      14.09
 C      -3.780907    -0.342075    -0.947389      70.57
 H      -4.664527    -1.054742    -1.366966      23.09
 O      -4.471212    -0.066581     0.404104     172.29
 H      -3.968641     0.150693     1.239340      23.62
 C      -2.467544    -0.973811    -0.991169      96.72
 H      -2.209923    -0.885766    -1.988816      28.32
 C      -2.507815    -2.461714    -0.437802     102.88
 O      -3.687612    -3.253092    -1.025347     240.74
 H      -3.293760    -3.881013    -1.638876      29.76
 H      -2.892086    -2.303693     0.595414      24.30
 H      -1.588103    -3.202033    -0.712641      21.10
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 C       2.034745    -0.729317    -1.663059      42.46
 H       2.649827    -1.373705    -2.259435      24.09
 C       1.961305     0.994543     0.068014      68.97
 H       2.401802     1.718102     0.553050      24.52
 C       0.576074     0.725097     0.354822       5.93
 O      -0.153635     1.356384     1.335887     184.54
 C       0.204885     2.768528     1.741928      71.57
 H      -0.750950     3.131262     2.373654      22.15
 H       1.310156     2.703853     2.364630      20.87
 H       0.106462     3.528211     0.792128      23.80
 C      -0.110206    -0.245177    -0.470000       5.52
 O      -1.518532    -0.294207    -0.124909     168.24
 C       0.620444    -0.988859    -1.357404      61.16
 H       0.182052    -1.964110    -1.962896      21.52
 C       2.670609     0.290779    -0.883858      23.11
 C       4.101391     0.692973    -1.235748      62.34
 H       4.271293     0.455421    -2.496060      19.69
 O       4.252454     2.239795    -1.424847     201.44
 H       4.312705     2.702834    -0.501706      21.06
 C       5.232163     0.086815    -0.350141     104.30
 H       5.285741     0.287035     0.776590      22.68
 O       4.991712    -1.382341    -0.347773     330.54
 H       5.478128    -1.623231    -1.186878      28.00
 C       6.595440     0.482365    -0.890200     107.33
 O       6.793953     1.933312    -0.592176     222.33
 H       7.176294     1.961564     0.304621      27.66
 H       6.438798     0.330527    -1.905725      32.86
 H       7.575146     0.054194    -0.609329      30.37
55
name= lig-ACN-Water-frame_322
 C      -3.692278     0.849205    -3.172605      35.82
 H      -3.514077    -0.099043    -3.781231      25.31
 C      -4.161931     2.203273    -1.138146      66.02
 H      -4.204395     2.233800    -0.068256      24.04
 C      -4.265552     3.345044    -1.912570       9.76
 O      -4.522035     4.644855    -1.334866     212.68
 C      -4.772975     4.805205     0.067457     103.70
 H      -3.708853     4.695929     0.491950      25.81
 H      -5.572648     3.978058     0.405496      25.07
 H      -5.107782     5.756556     0.435955      24.62
 C      -4.285529     3.263132    -3.380094      10.16
 O      -4.748263     4.258438    -4.154107     175.22
 H      -4.919332     5.037766    -3.669092      24.94
 C      -3.763796     2.036973    -4.015613      42.28
 H      -3.800669     1.779442    -5.094839      21.34
 C      -3.740522     1.001931    -1.793761      34.99
 C      -3.898240    -0.276286    -0.978026      62.47
 H      -4.494931    -1.122927    -1.637693      23.22
 O      -4.469958    -0.119490     0.374494     183.02
 H      -3.641370     0.111832     0.794415      27.78
 C      -2.402454    -1.085637    -0.989072      69.66
 H      -1.948285    -1.147790    -1.956182      27.08
 C      -2.680530    -2.567379    -0.424373     106.87
 O      -3.779574    -3.323134    -1.046207     242.19
 H      -3.368614    -3.991445    -1.582610      28.98
 H      -2.556948    -2.595024     0.693528      26.51
 H      -1.561703    -3.048840    -0.618947      23.48
 C       1.989304    -0.733033    -1.601168      45.93
 H       2.584678    -1.445241    -2.138798      20.33
 C       1.885586     1.119160     0.001005      62.93
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 H       2.408247     1.834034     0.567855      19.91
 C       0.571485     0.824199     0.258024      15.26
 O      -0.177814     1.388078     1.304547     199.62
 C       0.170132     2.700874     1.738248      86.49
 H      -0.775365     3.108819     2.408871      21.37
 H       1.157644     2.849866     2.553402      21.87
 H       0.550468     3.356333     0.784069      22.42
 C      -0.123169    -0.240102    -0.381622       0.11
 O      -1.495298    -0.274848    -0.150794     138.78
 C       0.642593    -0.940066    -1.427883      63.64
 H       0.034279    -1.909991    -1.914663      20.31
 C       2.617967     0.411581    -1.031265      21.60
 C       4.104286     0.780270    -1.212135      70.20
 H       4.462782     0.161765    -2.273324      21.04
 O       4.270570     2.218029    -1.343671     213.93
 H       4.784008     2.527989    -0.490275      17.66
 C       5.209388     0.058368    -0.301238      67.58
 H       5.112265     0.514033     0.772274      22.14
 O       5.116287    -1.386265    -0.287881     356.51
 H       5.260374    -1.749115    -1.189429      27.85
 C       6.612975     0.526717    -1.006348      96.82
 O       6.881536     1.900855    -0.644013     263.34
 H       7.116319     1.916265     0.327388      32.35
 H       6.705465     0.560017    -2.019953      33.46
 H       7.221824    -0.314721    -0.573720      31.31
55
name= lig-ACN-Water-frame_323
 C      -3.597868     0.903773    -3.209357      38.25
 H      -3.735802    -0.187440    -3.579813      23.56
 C      -4.107397     2.207236    -1.216342      64.84
 H      -4.099411     2.243827    -0.222181      24.97
 C      -4.277781     3.394821    -1.973919      19.00
 O      -4.549655     4.595315    -1.418062     169.72
 C      -4.760416     4.723518     0.091230      88.35
 H      -3.819247     4.566985     0.824440      23.74
 H      -5.450770     3.921095     0.514779      25.04
 H      -5.262303     5.781884    -0.028429      22.24
 C      -4.281676     3.218274    -3.377694      28.35
 O      -4.795732     4.200415    -4.249354     142.98
 H      -4.590372     5.118184    -3.960307      24.36
 C      -3.864688     2.023866    -3.961405      77.95
 H      -3.772099     2.112188    -5.002368      25.72
 C      -3.772063     0.959706    -1.779850      -5.90
 C      -3.824917    -0.328102    -1.008174      67.18
 H      -4.750862    -0.972769    -1.538176      23.31
 O      -4.374218    -0.195029     0.281228     204.98
 H      -3.854731     0.084203     1.066129      24.20
 C      -2.509762    -1.202098    -0.936994      81.96
 H      -2.164029    -1.316465    -1.994526      26.37
 C      -2.682421    -2.665841    -0.393908     107.61
 O      -3.825879    -3.347871    -1.042736     183.61
 H      -3.422170    -4.077759    -1.671432      26.70
 H      -3.126426    -2.679977     0.624259      24.83
 H      -1.778418    -3.398216    -0.707313      22.31
 C       1.978331    -0.686207    -1.573106      55.15
 H       2.384551    -1.212052    -2.433420      16.50
 C       1.869453     1.261204    -0.110981      56.49
 H       2.350839     2.121498     0.474174      18.50
 C       0.519992     0.866067     0.252116       8.78
 O      -0.194009     1.415264     1.270217     214.25
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 C       0.179682     2.714820     1.754621      77.13
 H      -0.828247     3.274025     2.142970      21.63
 H       1.083912     2.459023     2.572375      21.55
 H       0.507717     3.454140     0.830370      22.08
 C      -0.122341    -0.201153    -0.468909      19.80
 O      -1.489245    -0.326467    -0.175410     147.53
 C       0.558383    -0.969292    -1.352077      68.34
 H       0.097731    -1.804662    -2.080096      20.47
 C       2.603106     0.500874    -1.035125      39.02
 C       4.075540     0.749594    -1.253267      85.46
 H       4.263213     0.493722    -2.498756      19.49
 O       4.300781     2.168563    -1.235995     224.69
 H       5.124357     2.436397    -0.826823      20.93
 C       5.212773     0.102883    -0.390808      75.61
 H       5.139333     0.442465     0.717740      22.20
 O       5.201064    -1.343653    -0.200314     316.65
 H       5.334079    -1.709684    -1.105188      30.33
 C       6.576237     0.522280    -0.988099     112.65
 O       7.016631     1.869590    -0.671873     237.33
 H       7.232388     1.988270     0.327648      28.64
 H       6.451047     0.366872    -1.994258      36.13
 H       7.491540    -0.060744    -0.690075      31.43
55
name= lig-ACN-Water-frame_324
 C      -3.589467     0.877235    -3.189384      48.27
 H      -3.107332     0.041458    -3.832696      20.95
 C      -3.963993     2.194813    -1.200671      61.90
 H      -4.207646     2.291018    -0.252502      20.58
 C      -4.307593     3.341047    -1.986342       8.53
 O      -4.588525     4.597577    -1.439442     206.94
 C      -4.778321     4.629192    -0.007147     103.59
 H      -3.669616     4.640349     0.551275      22.44
 H      -5.560974     3.950434     0.309559      24.89
 H      -5.188917     5.748307     0.359322      22.16
 C      -4.296971     3.281718    -3.416225      19.32
 O      -4.804391     4.183608    -4.351478     207.53
 H      -4.417803     5.184723    -4.237637      19.84
 C      -3.951580     2.042458    -3.963869      39.25
 H      -3.739050     1.923042    -4.973897      26.80
 C      -3.793857     0.928675    -1.833941      22.43
 C      -3.735700    -0.439423    -0.985275      83.48
 H      -4.450108    -1.204560    -1.659054      24.14
 O      -4.353338    -0.267961     0.305333     199.92
 H      -3.546089     0.159083     0.803886      24.35
 C      -2.503778    -1.276414    -0.982691      89.93
 H      -2.169520    -1.361819    -2.083108      26.53
 C      -2.749926    -2.754378    -0.324402     103.77
 O      -3.874676    -3.383117    -1.085806     198.96
 H      -3.450131    -3.959107    -1.821774      26.31
 H      -2.841866    -2.549102     0.766452      26.32
 H      -1.691801    -3.278491    -0.222742      24.46
 C       1.912516    -0.587489    -1.648974      58.13
 H       2.594983    -1.085215    -2.359133      19.90
 C       1.788769     1.335754    -0.159174      62.38
 H       2.277559     2.394434     0.201113      18.19
 C       0.532616     0.886081     0.193345      14.94
 O      -0.246793     1.450016     1.221311     182.55
 C       0.196601     2.780174     1.751677      83.79
 H      -0.729691     3.174838     2.338683      22.86
 H       1.066686     2.815587     2.653999      22.53
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 H       0.658435     3.495182     0.889656      22.07
 C      -0.205813    -0.158073    -0.529523       2.92
 O      -1.572794    -0.447488    -0.185666     151.43
 C       0.631366    -1.003612    -1.332163      60.46
 H       0.077031    -1.784954    -1.917010      22.94
 C       2.568983     0.454720    -0.956745      29.60
 C       4.063985     0.728903    -1.380634      72.04
 H       4.281425     0.196743    -2.519505      20.37
 O       4.316225     2.194016    -1.176419     200.20
 H       5.257811     2.246843    -0.992892      20.58
 C       5.214294     0.117358    -0.400111      95.79
 H       5.043215     0.670440     0.590840      21.35
 O       5.243808    -1.293995    -0.170485     278.61
 H       5.476817    -1.758445    -1.064442      25.19
 C       6.619419     0.472694    -0.976975      96.12
 O       7.098954     1.878343    -0.721904     193.34
 H       7.365552     1.877737     0.286331      28.86
 H       6.620548     0.544297    -2.026789      34.03
 H       7.274697    -0.372811    -0.625216      31.85
55
name= lig-ACN-Water-frame_325
 C      -3.613400     0.894124    -3.257883      58.27
 H      -2.967507     0.081624    -3.674437      28.58
 C      -3.947172     2.139046    -1.186716      36.42
 H      -3.941771     2.087131    -0.132873      24.57
 C      -4.302473     3.357209    -2.024398       9.48
 O      -4.643177     4.595230    -1.478935     201.13
 C      -4.786964     4.591645    -0.078072     103.41
 H      -3.765769     4.068760     0.415172      23.66
 H      -5.410485     3.808406     0.259912      26.69
 H      -5.163820     5.720125     0.274939      23.11
 C      -4.352541     3.277061    -3.477784       9.14
 O      -4.771316     4.229760    -4.429399     132.67
 H      -4.811462     5.241197    -4.098641      22.06
 C      -3.911158     2.002157    -4.031806      40.67
 H      -3.946422     1.996798    -5.091865      22.03
 C      -3.697260     0.844129    -1.772280      -8.18
 C      -3.829270    -0.483488    -1.055791      50.64
 H      -4.687037    -1.217958    -1.534524      20.61
 O      -4.292432    -0.331877     0.346544     137.01
 H      -3.685101     0.144018     1.018225      23.85
 C      -2.375436    -1.362981    -1.013623      75.90
 H      -1.814674    -1.615390    -2.022051      24.76
 C      -2.790129    -2.699929    -0.305070     107.07
 O      -3.839341    -3.420407    -1.082665     226.43
 H      -3.384806    -3.958513    -1.686574      30.93
 H      -3.401393    -2.688518     0.607612      24.13
 H      -1.981116    -3.474085    -0.439331      24.41
 C       1.947380    -0.573619    -1.688908      52.93
 H       2.422429    -1.398410    -2.257920      19.33
 C       1.753699     1.296941    -0.195621      29.78
 H       2.180642     2.326887     0.376623      20.13
 C       0.374467     0.924982     0.136838       8.31
 O      -0.258047     1.569845     1.187516     208.05
 C       0.187163     2.835092     1.757393      96.88
 H      -0.683002     3.293828     2.259754      24.50
 H       1.192583     2.547904     2.379902      22.90
 H       0.364416     3.574102     0.837961      23.91
 C      -0.237572    -0.214481    -0.510779      14.30
 O      -1.540766    -0.557815    -0.169035     176.37
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 C       0.593732    -0.982423    -1.389809      50.02
 H       0.328032    -1.929375    -1.710417      24.31
 C       2.612744     0.481063    -1.019421      39.80
 C       4.059443     0.764182    -1.309425      87.49
 H       4.261441     0.555074    -2.529410      19.59
 O       4.292103     2.164402    -1.252213     260.66
 H       5.247568     2.442584    -0.988088      18.15
 C       5.192259     0.147109    -0.437739      95.52
 H       5.042100     0.583560     0.589032      21.23
 O       5.236042    -1.280423    -0.167321     288.71
 H       5.293987    -1.733543    -1.120829      24.52
 C       6.687487     0.483736    -1.018793      94.22
 O       7.114807     1.805152    -0.738926     259.39
 H       7.262917     2.050247     0.245031      29.36
 H       6.789888     0.170135    -2.078240      30.09
 H       7.388193    -0.179750    -0.477401      29.39
55
name= lig-ACN-Water-frame_326
 C      -3.563091     0.854442    -3.251503      38.86
 H      -3.675380    -0.075928    -3.780363      23.91
 C      -4.010064     2.136911    -1.285905      67.18
 H      -3.936277     2.385469    -0.177866      24.10
 C      -4.272828     3.271235    -2.068298       7.74
 O      -4.686380     4.558131    -1.575550     157.32
 C      -4.791275     4.478514    -0.058469     107.31
 H      -3.733840     4.424761     0.615811      23.62
 H      -5.664555     4.025719     0.198091      28.07
 H      -4.983041     5.661158     0.179596      24.94
 C      -4.361849     3.179323    -3.508960      27.04
 O      -4.729596     4.270424    -4.418170     139.78
 H      -4.926467     5.001491    -3.885802      25.35
 C      -3.894122     2.032457    -4.074119      40.84
 H      -3.702377     1.900431    -5.155169      24.45
 C      -3.659957     0.904118    -1.875161      20.95
 C      -3.763246    -0.502023    -1.039423      63.09
 H      -4.697075    -0.979962    -1.563320      24.46
 O      -4.246288    -0.401085     0.336103     195.16
 H      -3.541469     0.079626     0.819294      26.66
 C      -2.446364    -1.412250    -0.983009      70.85
 H      -1.988924    -1.511891    -2.085413      25.37
 C      -2.825496    -2.748036    -0.338264     120.51
 O      -3.808305    -3.449848    -1.126777     249.79
 H      -3.347386    -4.164054    -1.648800      27.27
 H      -3.116545    -2.300764     0.620377      25.97
 H      -1.940942    -3.251439     0.079822      26.88
 C       1.968354    -0.687901    -1.638178      37.21
 H       2.653090    -1.218256    -2.326443      20.97
 C       1.693651     1.189255    -0.205588      53.23
 H       2.264946     2.002037     0.505972      19.59
 C       0.355205     0.976678     0.062973      14.75
 O      -0.362897     1.650139     1.136761     180.78
 C       0.188624     2.886924     1.679973     110.56
 H      -0.426819     3.093001     2.499542      26.29
 H       1.258433     2.780990     2.257286      23.63
 H       0.343337     3.747057     0.927925      24.33
 C      -0.188274    -0.241395    -0.490333       4.67
 O      -1.472556    -0.655607    -0.099121     148.85
 C       0.583539    -0.949542    -1.412703      72.31
 H       0.244132    -1.814136    -1.755109      23.94
 C       2.525375     0.514950    -1.109641      25.07
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 C       4.106128     0.807978    -1.298481      67.33
 H       4.275771     0.227914    -2.419477      23.16
 O       4.239870     2.246551    -1.358794     216.81
 H       5.088068     2.482336    -0.836892      18.55
 C       5.279749     0.130386    -0.446435      91.95
 H       5.288580     0.586390     0.557014      23.75
 O       5.155579    -1.292148    -0.224263     331.06
 H       5.247145    -1.803072    -1.087407      28.19
 C       6.695102     0.402316    -0.942397     100.72
 O       7.085017     1.820048    -0.795374     183.29
 H       7.252979     1.894981     0.158215      31.04
 H       6.729028     0.247782    -2.081201      31.44
 H       7.357908    -0.263009    -0.398258      32.56
55
name= lig-ACN-Water-frame_327
 C      -3.611422     0.805405    -3.337310      61.04
 H      -3.610986    -0.116282    -3.826307      26.19
 C      -4.005260     2.169201    -1.359353      53.18
 H      -4.184129     2.131708    -0.161295      23.28
 C      -4.357040     3.271442    -2.181409      29.81
 O      -4.672214     4.419836    -1.549608     216.41
 C      -4.846159     4.574899    -0.126314     112.63
 H      -3.855905     3.928247     0.301438      22.85
 H      -5.509097     3.865691     0.253069      27.41
 H      -5.103212     5.660852     0.142862      24.73
 C      -4.312939     3.197363    -3.571747       8.49
 O      -4.670173     4.217394    -4.306586     155.81
 H      -4.747634     5.114786    -3.884713      26.41
 C      -3.817040     1.931433    -4.121795      16.85
 H      -3.779183     1.876004    -5.262319      19.28
 C      -3.679494     0.885439    -1.887364      14.42
 C      -3.663379    -0.429263    -1.039133      84.35
 H      -4.265504    -1.216536    -1.654409      25.28
 O      -4.207776    -0.403103     0.276208     171.07
 H      -3.676100     0.054154     0.972739      22.97
 C      -2.500914    -1.347778    -1.019202      61.24
 H      -2.059955    -1.458074    -2.135483      26.42
 C      -2.810207    -2.735629    -0.266468     105.24
 O      -3.762243    -3.502707    -1.157678     172.51
 H      -3.174416    -4.226676    -1.675356      24.72
 H      -3.507515    -2.728731     0.546274      24.59
 H      -1.959079    -3.345582    -0.223041      25.86
 C       1.976514    -0.712234    -1.646846      40.57
 H       2.455699    -1.392330    -2.353214      19.95
 C       1.734843     1.226032    -0.154232      43.98
 H       2.279959     2.092027     0.372032      18.80
 C       0.342580     0.952554     0.102991       3.73
 O      -0.438645     1.680712     1.003434     190.17
 C       0.208183     2.936325     1.659615     100.76
 H      -0.409717     3.207829     2.447510      26.01
 H       1.299637     2.653600     1.874147      23.16
 H       0.054772     3.706239     0.889087      25.06
 C      -0.216027    -0.224519    -0.503249     -25.32
 O      -1.441576    -0.753968    -0.029057     119.24
 C       0.639086    -1.048177    -1.409732      41.41
 H       0.074398    -1.702141    -1.963317      23.01
 C       2.551976     0.425995    -1.099243      33.45
 C       4.053927     0.799027    -1.360529      66.34
 H       4.456118     0.491334    -2.476130      22.35
 O       4.207740     2.334476    -1.468080     241.46
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 H       4.747940     2.664494    -0.764983      22.76
 C       5.275857     0.109987    -0.332095      81.70
 H       5.168333     0.502370     0.666269      23.89
 O       5.037686    -1.318033    -0.301344     366.86
 H       5.290638    -1.719531    -1.154984      28.71
 C       6.715653     0.363539    -0.926854      97.91
 O       7.049386     1.821717    -0.840298     233.04
 H       7.132039     2.178974     0.063874      32.00
 H       6.839039     0.121044    -2.089555      31.72
 H       7.409858    -0.328754    -0.469376      32.43
55
name= lig-ACN-Water-frame_328
 C      -3.665724     0.718250    -3.361438      62.55
 H      -3.091839    -0.066880    -3.707710      29.25
 C      -4.012661     2.057120    -1.390383      66.75
 H      -4.287384     2.143348    -0.198755      21.00
 C      -4.378873     3.158129    -2.098508       8.66
 O      -4.725394     4.445921    -1.595571     200.10
 C      -4.857332     4.502361    -0.184509     124.75
 H      -3.837626     4.560310     0.529998      23.06
 H      -5.759994     4.076548     0.162736      26.46
 H      -5.058129     5.585067    -0.080289      25.61
 C      -4.169265     3.105738    -3.558553       8.77
 O      -4.632968     4.249303    -4.338208     135.89
 H      -4.303092     5.095800    -3.766778      21.23
 C      -3.818438     1.922520    -4.180795      45.94
 H      -3.764291     1.820297    -5.320490      20.70
 C      -3.705070     0.837983    -1.962453      25.11
 C      -3.661594    -0.407034    -1.112480      83.79
 H      -4.526728    -0.929322    -1.566337      21.80
 O      -4.256031    -0.342597     0.230288     166.75
 H      -3.633541     0.204718     0.852458      23.39
 C      -2.358901    -1.311597    -0.900986      83.62
 H      -1.830508    -1.681105    -1.889290      23.43
 C      -2.855868    -2.755315    -0.360823     119.75
 O      -3.711272    -3.562756    -1.180607     248.32
 H      -3.126976    -4.082396    -1.849613      24.41
 H      -3.029442    -2.571638     0.686377      26.15
 H      -1.926363    -3.151920    -0.213681      26.82
 C       1.964564    -0.727490    -1.700070      56.67
 H       2.591513    -1.363288    -2.316370      18.50
 C       1.798492     1.230418    -0.176883      53.71
 H       2.119855     2.203717     0.071118      19.68
 C       0.429174     0.871813     0.141861      -3.84
 O      -0.470305     1.740456     0.900613     186.85
 C       0.137673     2.899879     1.530903     120.25
 H      -0.340383     3.008194     2.477705      26.18
 H       1.202818     2.739884     1.844486      24.56
 H       0.139022     3.753150     0.918210      26.47
 C      -0.190754    -0.295578    -0.519414      11.77
 O      -1.412554    -0.803721    -0.020558     199.14
 C       0.569986    -1.064958    -1.343992      50.52
 H       0.340156    -2.030524    -1.848813      21.07
 C       2.632931     0.386526    -0.965753      15.93
 C       4.078162     0.880214    -1.358484      63.59
 H       4.134324     0.434952    -2.440811      19.03
 O       4.149340     2.344513    -1.542326     264.57
 H       4.557734     2.686689    -0.709538      21.94
 C       5.150520     0.096541    -0.385526      97.37
 H       5.040989     0.393367     0.640305      21.76
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 O       4.918621    -1.333368    -0.345592     358.21
 H       5.056813    -1.631020    -1.299639      25.18
 C       6.708594     0.424871    -0.878487      96.16
 O       7.035498     1.790769    -0.898693     310.05
 H       6.916288     1.983729     0.094749      32.37
 H       6.576661    -0.035946    -1.972764      32.23
 H       7.474082    -0.022509    -0.274692      29.62
55
name= lig-ACN-Water-frame_329
 C      -3.565534     0.710235    -3.432304      51.99
 H      -3.351829    -0.197533    -3.981607      20.00
 C      -4.113659     1.963777    -1.296895      35.43
 H      -4.021578     1.960324    -0.114639      25.89
 C      -4.301397     3.161121    -2.151899      14.92
 O      -4.746126     4.382149    -1.699151     162.37
 C      -4.927541     4.620558    -0.181141     104.55
 H      -3.923866     4.125786     0.364338      23.36
 H      -5.582346     3.816769     0.200596      24.58
 H      -5.193780     5.606357    -0.023146      26.77
 C      -4.173021     3.132076    -3.543677      12.84
 O      -4.509691     4.223871    -4.336817     190.03
 H      -4.335901     5.154935    -4.018380      21.81
 C      -3.836741     1.860970    -4.175344      21.27
 H      -3.515939     1.885088    -5.246292      26.54
 C      -3.719131     0.775717    -2.011888      17.20
 C      -3.703520    -0.523262    -1.119246      71.73
 H      -4.159817    -1.342910    -1.644829      28.98
 O      -4.323978    -0.220730     0.160652     106.66
 H      -3.701111     0.252606     0.856019      22.50
 C      -2.350103    -1.397461    -0.961944      68.45
 H      -1.865685    -1.278000    -1.986362      27.37
 C      -2.696580    -2.766840    -0.384730     119.06
 O      -3.697766    -3.548997    -1.163353     201.03
 H      -3.213134    -4.104261    -1.771292      28.89
 H      -3.433622    -2.630358     0.383072      25.96
 H      -1.938096    -3.380858    -0.250852      28.49
 C       1.991325    -0.676190    -1.572883      29.48
 H       2.545575    -1.259467    -2.281928      24.47
 C       1.749819     1.206189    -0.186664      68.17
 H       2.120272     2.073631     0.067199      25.23
 C       0.456763     0.834078     0.109346      27.87
 O      -0.442607     1.710536     0.754670     213.99
 C       0.100889     2.868049     1.465997     123.68
 H      -0.615448     3.104935     2.278393      26.38
 H       1.089112     2.682052     1.780030      27.00
 H       0.050948     3.741744     0.869519      27.94
 C      -0.104582    -0.344837    -0.394342     -12.97
 O      -1.383093    -0.764459     0.053701     129.61
 C       0.704631    -1.108183    -1.383263      70.52
 H       0.158674    -2.150286    -1.467452      18.37
 C       2.614139     0.366503    -0.975875      41.66
 C       4.034829     0.824104    -1.359200      94.11
 H       4.364575     0.481383    -2.374249      26.03
 O       4.098927     2.302444    -1.530244     213.53
 H       4.731616     2.726990    -0.808877      21.83
 C       5.105748     0.170516    -0.473854      98.85
 H       4.931754     0.542229     0.532521      24.66
 O       4.795120    -1.291374    -0.400098     298.87
 H       4.826390    -1.813059    -1.308248      28.31
 C       6.553876     0.374892    -0.819803      98.80
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 O       6.995676     1.817250    -0.931614     253.24
 H       7.272485     2.313517    -0.074365      30.17
 H       7.025869     0.074546    -1.865454      30.56
 H       7.033316    -0.296162    -0.117954      31.41
55
name= lig-ACN-Water-frame_330
 C      -3.509981     0.722403    -3.409946      32.58
 H      -3.604538    -0.249184    -3.972728      23.07
 C      -4.118017     1.940762    -1.420016      65.10
 H      -4.284193     2.020658    -0.335148      25.28
 C      -4.264855     3.122775    -2.101950      12.16
 O      -4.779344     4.384657    -1.674856     198.58
 C      -4.945966     4.573738    -0.294411     116.96
 H      -3.834360     4.514696     0.215403      24.65
 H      -5.827118     3.974479     0.126948      24.89
 H      -5.199316     5.547888    -0.096326      28.94
 C      -4.182610     3.081655    -3.571295      28.33
 O      -4.353491     4.192006    -4.372619     122.10
 H      -4.432889     4.886323    -3.774594      25.24
 C      -3.767415     1.927071    -4.171226      50.89
 H      -3.736724     1.922945    -5.255341      24.29
 C      -3.748143     0.657849    -1.984856       4.01
 C      -3.683183    -0.634394    -1.121530      96.04
 H      -4.436597    -1.249289    -1.462496      30.87
 O      -4.398783    -0.155726     0.068413     153.87
 H      -3.772782    -0.028636     0.808781      28.43
 C      -2.323727    -1.342178    -1.020941      70.73
 H      -1.843851    -1.491033    -1.996172      28.30
 C      -2.642712    -2.835671    -0.359345     113.48
 O      -3.687097    -3.505448    -1.179533     241.26
 H      -3.195176    -4.159680    -1.698878      28.43
 H      -2.877731    -2.543044     0.656147      28.72
 H      -1.808333    -3.293823    -0.139944      29.68
 C       2.085459    -0.799129    -1.564124      80.04
 H       2.665793    -1.387683    -2.274151      19.16
 C       1.801265     1.235685    -0.174139      70.33
 H       2.121971     2.067129     0.264426      23.10
 C       0.434825     0.832381     0.055413      -7.54
 O      -0.465923     1.671615     0.668466     207.12
 C       0.050366     2.873814     1.404595     109.34
 H      -0.800626     3.106285     2.160830      25.31
 H       0.909533     2.707438     1.978050      27.44
 H       0.161737     3.565559     0.615526      26.51
 C      -0.043665    -0.470849    -0.333362      26.66
 O      -1.372552    -0.713719     0.081063     139.60
 C       0.707796    -1.165670    -1.196222      80.26
 H       0.512907    -2.042570    -2.003575      21.52
 C       2.560233     0.474254    -1.036367      23.98
 C       3.964944     0.798962    -1.474736      93.97
 H       4.013074     0.381240    -2.468932      27.09
 O       4.072658     2.262034    -1.455031     195.47
 H       4.924314     2.421258    -0.999384      26.69
 C       5.001589     0.195272    -0.480825      90.84
 H       4.869363     0.614896     0.536337      26.77
 O       4.694393    -1.197696    -0.408435     318.49
 H       4.907309    -1.476421    -1.403827      28.89
 C       6.527803     0.372756    -0.803388      87.83
 O       6.957464     1.823957    -0.932166     197.77
 H       7.272785     1.887349    -0.015288      29.97
 H       6.615536    -0.300698    -1.769340      32.70
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 H       7.133948     0.082836     0.070668      29.81
55
name= lig-ACN-Water-frame_331
 C      -3.582130     0.689872    -3.410065      66.21
 H      -3.076770    -0.214375    -3.943848      27.90
 C      -4.093586     1.898961    -1.441647      59.56
 H      -4.482526     1.860744    -0.513549      25.78
 C      -4.322695     3.120157    -2.215815      21.43
 O      -4.773976     4.344350    -1.714829     210.26
 C      -4.956800     4.591250    -0.308451     117.74
 H      -4.036185     4.404388     0.450794      24.67
 H      -5.724057     3.844668     0.146461      25.20
 H      -5.287978     5.579129    -0.314237      28.88
 C      -4.096549     3.084654    -3.553129      24.01
 O      -4.216019     4.185346    -4.370580     156.93
 H      -4.550874     5.079906    -3.986542      23.46
 C      -3.666433     1.858207    -4.159294      44.83
 H      -3.656253     1.782124    -5.209754      23.36
 C      -3.722744     0.690338    -2.054960      24.39
 C      -3.759785    -0.549832    -1.181382      72.91
 H      -4.178535    -1.320403    -1.667661      27.18
 O      -4.419382    -0.196341     0.067013     172.98
 H      -3.806009     0.140465     0.727710      26.56
 C      -2.299005    -1.411394    -0.872263      86.08
 H      -1.808348    -1.411104    -1.806654      27.06
 C      -2.579194    -2.776397    -0.366195     129.12
 O      -3.625715    -3.452758    -1.125504     218.95
 H      -3.130672    -4.098897    -1.784284      26.52
 H      -2.971242    -2.874853     0.616244      27.34
 H      -1.833932    -3.327233    -0.632461      28.50
 C       2.053267    -0.822310    -1.500057      49.49
 H       2.658265    -1.402031    -2.212893      23.03
 C       1.786133     1.244144    -0.177124      60.75
 H       2.200944     2.203655     0.137826      21.19
 C       0.481503     0.820864     0.060492       9.34
 O      -0.532297     1.655793     0.685106     188.52
 C      -0.036369     2.851526     1.305877     117.20
 H      -0.966738     3.344446     1.856249      24.78
 H       0.701903     2.608529     1.983802      28.48
 H       0.434725     3.708674     0.739152      25.68
 C      -0.048185    -0.460410    -0.303260     -12.61
 O      -1.434964    -0.709249    -0.014472     152.59
 C       0.847534    -1.342721    -1.143992      62.34
 H       0.149138    -2.186490    -1.590208      19.35
 C       2.529981     0.423256    -1.146081      23.73
 C       3.897026     0.884984    -1.553428     101.57
 H       4.232296     0.552684    -2.491812      27.35
 O       4.093204     2.269380    -1.408324     233.75
 H       5.016604     2.397386    -1.294422      26.94
 C       4.910077     0.220528    -0.455261      78.86
 H       4.514297     0.672462     0.507455      26.07
 O       4.652216    -1.157783    -0.377766     357.45
 H       4.720367    -1.715752    -1.211319      27.48
 C       6.475089     0.409780    -0.777006      96.57
 O       6.907274     1.757725    -0.935066     305.96
 H       7.121326     2.208553    -0.119953      33.09
 H       6.855658    -0.052476    -1.780740      29.31
 H       7.059049    -0.248688    -0.037649      28.56
55
name= lig-ACN-Water-frame_332
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 C      -3.524681     0.604979    -3.497118      50.49
 H      -3.000463    -0.335594    -3.996331      23.89
 C      -4.170411     1.970647    -1.418779      78.02
 H      -4.312504     1.974450    -0.448686      25.79
 C      -4.361465     3.052991    -2.209744      22.98
 O      -4.741570     4.311916    -1.770776     196.52
 C      -5.003478     4.580678    -0.275144     106.58
 H      -3.949213     4.458543     0.141178      23.93
 H      -5.816775     3.834924     0.108060      23.82
 H      -5.318686     5.598659    -0.026845      25.79
 C      -3.962140     3.081187    -3.637430      18.87
 O      -4.113259     4.196382    -4.420230     152.91
 H      -4.223486     5.124921    -3.868456      19.52
 C      -3.630957     1.829362    -4.226391      54.43
 H      -3.140576     1.897936    -5.164539      23.87
 C      -3.709282     0.746424    -2.044087      17.52
 C      -3.702176    -0.530544    -1.160702      83.36
 H      -4.369300    -1.108075    -1.599306      26.21
 O      -4.416117    -0.310109     0.092611     148.57
 H      -3.853346     0.290540     0.685252      25.38
 C      -2.380706    -1.310298    -0.898309      85.70
 H      -2.010721    -1.511524    -1.852381      28.47
 C      -2.509311    -2.856618    -0.363117     120.30
 O      -3.615289    -3.420373    -1.109691     211.48
 H      -3.175811    -3.972133    -1.899033      24.89
 H      -2.655485    -2.807629     0.693209      27.99
 H      -1.602011    -3.245257    -0.327762      29.25
 C       2.026830    -0.880783    -1.530486      60.48
 H       2.632969    -1.532918    -2.207172      17.52
 C       1.737077     1.192193    -0.303130      56.80
 H       2.171185     2.256550    -0.041155      19.36
 C       0.409848     0.808338     0.138937       6.11
 O      -0.556723     1.616062     0.679455     207.57
 C      -0.092049     2.889626     1.291133     101.05
 H      -1.084578     3.502919     1.557287      24.43
 H       0.375140     2.669700     2.184038      27.85
 H       0.488326     3.288733     0.367045      23.60
 C      -0.043828    -0.459567    -0.381962       1.36
 O      -1.398607    -0.647485    -0.023008     142.97
 C       0.743212    -1.386936    -0.987824      65.56
 H       0.628332    -2.338220    -1.054257      24.47
 C       2.493862     0.439505    -1.168454      38.56
 C       3.962359     0.886370    -1.539143      85.23
 H       4.097432     0.621714    -2.515227      22.67
 O       4.098809     2.391628    -1.411615     219.95
 H       5.111130     2.539185    -1.426989      19.56
 C       4.865824     0.227382    -0.528772     103.02
 H       4.773096     0.719608     0.500519      22.35
 O       4.622957    -1.231581    -0.285098     343.33
 H       4.808926    -1.574464    -1.146825      27.90
 C       6.360580     0.377914    -0.764686      87.83
 O       6.872336     1.780078    -0.934004     327.59
 H       6.927669     2.162002     0.023209      32.24
 H       6.449521    -0.089781    -1.782823      30.51
 H       6.943216    -0.165711     0.087975      27.75
55
name= lig-ACN-Water-frame_333
 C      -3.426981     0.686554    -3.419459      38.65
 H      -3.357466    -0.392964    -3.858959      23.81
 C      -4.187743     1.923673    -1.448578      36.41
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 H      -4.285551     2.082768    -0.425488      27.48
 C      -4.336415     3.122545    -2.281062      17.85
 O      -4.775187     4.391090    -1.747535     158.04
 C      -4.956658     4.476175    -0.362902     120.76
 H      -4.106885     4.331866     0.357409      25.04
 H      -5.796564     3.799433     0.064619      23.79
 H      -5.280139     5.603316    -0.388928      25.13
 C      -3.945232     3.008480    -3.650630      23.41
 O      -4.011806     4.204863    -4.459980     141.78
 H      -3.970275     4.990901    -3.895964      25.76
 C      -3.502926     1.832101    -4.300673      73.65
 H      -3.228256     1.859554    -5.360623      28.62
 C      -3.713823     0.712699    -2.046763      15.18
 C      -3.701946    -0.537815    -1.085880      73.90
 H      -4.167111    -1.262444    -1.594207      31.26
 O      -4.380517    -0.397531     0.155445     163.51
 H      -3.857874     0.035511     0.926886      23.89
 C      -2.338823    -1.346332    -1.023221      74.83
 H      -1.843487    -1.241414    -1.923666      30.68
 C      -2.497344    -2.755801    -0.327568     120.34
 O      -3.581159    -3.460111    -1.104368     196.73
 H      -3.130226    -3.965865    -1.790151      29.79
 H      -2.918616    -2.710035     0.640881      27.79
 H      -1.729681    -3.357695    -0.574342      28.36
 C       1.979093    -0.914610    -1.517151      55.52
 H       2.598396    -1.704787    -1.988593      22.31
 C       1.632478     1.224394    -0.390574      60.47
 H       2.048212     2.270162     0.108734      24.33
 C       0.412686     0.787739     0.058219      24.82
 O      -0.588774     1.597009     0.742392     181.97
 C      -0.165294     2.894173     1.215422     116.30
 H      -1.118014     3.541029     1.207365      26.46
 H       0.317209     2.931996     2.212351      27.83
 H       0.696513     3.592348     0.670514      25.11
 C      -0.145550    -0.402810    -0.343919       6.10
 O      -1.438508    -0.598887     0.000985     132.78
 C       0.804165    -1.312320    -0.930081      69.51
 H       0.296180    -2.176733    -1.055911      26.27
 C       2.471411     0.398286    -1.221419      20.50
 C       3.890263     0.919438    -1.532456      92.28
 H       4.230341     0.606238    -2.414752      28.59
 O       4.071004     2.422139    -1.455928     192.81
 H       5.082269     2.624605    -1.233597      20.08
 C       4.866155     0.175212    -0.436330      86.17
 H       4.460547     0.643934     0.541452      25.56
 O       4.619231    -1.238899    -0.234981     334.13
 H       4.825321    -1.820623    -0.966465      30.04
 C       6.339692     0.354758    -0.855975     108.16
 O       6.795563     1.782995    -0.908209     232.74
 H       7.094150     1.969466     0.042893      27.77
 H       6.715100    -0.238868    -1.674033      30.75
 H       6.961865    -0.060548     0.048042      27.98
55
name= lig-ACN-Water-frame_334
 C      -3.379406     0.708637    -3.374081      34.16
 H      -3.137821    -0.242252    -3.945478      26.47
 C      -4.162427     1.993217    -1.521665      74.45
 H      -4.545478     1.866434    -0.479078      25.38
 C      -4.274891     3.126234    -2.305518      29.85
 O      -4.728606     4.348764    -1.844721     221.21
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 C      -4.965808     4.446488    -0.389809     111.27
 H      -4.021877     4.194482     0.121387      27.04
 H      -5.828477     3.731012    -0.138791      25.62
 H      -5.276825     5.523591     0.036772      25.69
 C      -3.957382     3.097579    -3.691995      13.86
 O      -3.898399     4.165956    -4.469993     150.18
 H      -4.310995     4.906280    -4.076342      27.98
 C      -3.409645     1.832311    -4.195948      30.04
 H      -3.465816     1.557602    -5.278240      17.12
 C      -3.738303     0.716365    -1.961493      21.82
 C      -3.703817    -0.624992    -1.147577      77.29
 H      -4.368632    -1.255737    -1.578662      27.44
 O      -4.334259    -0.468021     0.235484     165.56
 H      -3.645880    -0.038814     0.779464      28.28
 C      -2.236637    -1.291541    -0.975577      96.20
 H      -1.789525    -1.464379    -1.918993      29.11
 C      -2.568493    -2.696034    -0.458036     125.45
 O      -3.545374    -3.521104    -1.088219     259.63
 H      -3.071864    -4.063858    -1.700381      29.04
 H      -2.813937    -2.458303     0.562716      28.45
 H      -1.610517    -3.079710    -0.169782      27.50
 C       2.011375    -0.886011    -1.436165      99.33
 H       2.627291    -1.601988    -2.000607      19.74
 C       1.620107     1.279470    -0.451499      43.96
 H       2.152285     2.374035    -0.212444      18.94
 C       0.301821     0.935622    -0.002724      13.59
 O      -0.526116     1.617232     0.806449     216.27
 C      -0.236452     2.991052     1.189966     101.60
 H      -1.196614     3.570476     1.134018      26.20
 H      -0.028417     2.828219     2.261996      25.76
 H       0.653439     3.338776     0.362714      20.99
 C      -0.150257    -0.382843    -0.284275       2.32
 O      -1.558659    -0.623841    -0.005283     199.38
 C       0.675027    -1.312792    -0.970711      86.07
 H       0.430260    -2.282620    -1.420281      21.26
 C       2.423865     0.443351    -1.252687      33.87
 C       3.866250     0.877109    -1.514759     103.54
 H       4.119035     0.594437    -2.423604      27.47
 O       3.982904     2.333660    -1.480456     227.46
 H       4.876178     2.441300    -1.098145      24.01
 C       4.814781     0.152583    -0.420873      84.06
 H       4.899281     0.630667     0.621934      24.24
 O       4.613745    -1.247719    -0.186868     326.03
 H       4.787159    -1.601891    -1.156447      26.53
 C       6.428606     0.350724    -0.798262      92.96
 O       6.717938     1.754869    -0.890300     288.89
 H       7.059986     2.094752    -0.061935      32.01
 H       6.488686     0.086463    -1.809472      32.23
 H       7.039044    -0.324385    -0.072886      29.30
55
name= lig-ACN-Water-frame_335
 C      -3.337626     0.641699    -3.317484      83.12
 H      -2.802081    -0.223462    -3.648742      25.07
 C      -4.179045     1.956591    -1.462252      49.70
 H      -4.752682     2.204167    -0.460315      21.03
 C      -4.223813     3.124778    -2.305341      29.16
 O      -4.693705     4.369650    -1.902154     168.17
 C      -4.953680     4.366213    -0.440063     121.66
 H      -4.099839     4.024397     0.080383      25.84
 H      -5.851369     3.756553    -0.106703      24.35
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 H      -5.105805     5.583193    -0.241220      24.76
 C      -3.831585     3.054139    -3.673067      14.53
 O      -3.830365     4.211196    -4.541662     101.40
 H      -4.387754     4.992385    -4.110733      21.77
 C      -3.466614     1.830002    -4.091223      51.51
 H      -3.015615     1.914644    -5.141297      24.43
 C      -3.715055     0.708540    -1.981616      23.29
 C      -3.740013    -0.595794    -1.153042      70.80
 H      -4.318695    -1.318410    -1.675390      26.72
 O      -4.243684    -0.526494     0.205847     183.84
 H      -3.757946     0.063917     0.792692      26.64
 C      -2.391461    -1.311560    -1.088444      60.62
 H      -1.746927    -1.101893    -1.941677      26.40
 C      -2.550176    -2.697951    -0.369525     108.08
 O      -3.482337    -3.595473    -1.099336     165.75
 H      -3.019298    -4.145721    -1.849454      26.02
 H      -3.218753    -2.556639     0.461569      24.62
 H      -1.646723    -3.341418    -0.311737      23.94
 C       1.915885    -0.870585    -1.365099      25.41
 H       2.548988    -1.527649    -1.955236      21.81
 C       1.565786     1.401063    -0.498603      63.27
 H       1.901270     2.532115    -0.402411      16.71
 C       0.300032     0.962953    -0.058712       5.62
 O      -0.521240     1.682820     0.876468     207.06
 C      -0.316416     3.069347     1.177143     109.41
 H      -1.223016     3.604510     0.953838      27.53
 H       0.098243     3.430898     2.253108      23.80
 H       0.598724     3.696190     0.544575      21.78
 C      -0.198006    -0.390379    -0.312400       4.92
 O      -1.510902    -0.598608     0.024570     149.29
 C       0.641944    -1.258201    -1.094281      83.85
 H       0.171652    -2.338821    -1.243429      19.95
 C       2.376675     0.471446    -1.170894      39.17
 C       3.863644     0.755912    -1.481218     105.43
 H       4.123446     0.361909    -2.336961      24.07
 O       3.917981     2.216421    -1.466326     230.85
 H       4.804309     2.469630    -1.277646      25.24
 C       4.953308     0.173914    -0.395599      67.01
 H       4.490693     0.688191     0.511681      20.60
 O       4.599174    -1.249241    -0.200013     372.07
 H       4.634655    -1.852943    -1.052882      29.09
 C       6.340201     0.321933    -0.831196     118.63
 O       6.706358     1.780193    -0.836850     356.61
 H       6.717463     1.949627     0.136599      32.14
 H       6.471321    -0.100886    -1.773142      32.71
 H       7.163976    -0.155104    -0.233194      28.92
55
name= lig-ACN-Water-frame_336
 C      -3.286782     0.638247    -3.286516      35.83
 H      -2.891405    -0.209773    -3.738794      22.27
 C      -4.237374     1.949253    -1.465581      67.77
 H      -4.486811     1.753599    -0.292933      20.68
 C      -4.202480     3.123732    -2.296207      26.03
 O      -4.663864     4.350656    -1.861157     257.88
 C      -4.922220     4.392088    -0.512505     121.85
 H      -4.193492     4.055926     0.144437      25.43
 H      -5.912935     3.910581    -0.310903      25.20
 H      -5.115634     5.601917    -0.260420      24.76
 C      -3.762180     3.124965    -3.619420      20.58
 O      -3.802688     4.151003    -4.515947     231.69
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 H      -3.636994     5.169838    -4.112752      19.97
 C      -3.369895     1.751699    -4.189765      30.88
 H      -2.729565     1.617980    -5.134608      23.24
 C      -3.752761     0.731804    -1.915332      37.92
 C      -3.749551    -0.567005    -1.125109     107.33
 H      -4.469814    -1.182266    -1.643462      27.07
 O      -4.246664    -0.550625     0.165704     221.61
 H      -3.622242     0.011777     0.701967      24.97
 C      -2.413403    -1.347293    -1.053019      59.39
 H      -2.020223    -1.585539    -2.113867      25.59
 C      -2.596799    -2.757126    -0.366948     105.64
 O      -3.429821    -3.690252    -1.148306     205.73
 H      -2.794277    -3.978432    -1.953868      24.31
 H      -2.825990    -2.581740     0.697075      25.18
 H      -1.464239    -3.067876    -0.153428      23.30
 C       1.875422    -0.832876    -1.411195      31.60
 H       2.546436    -1.602465    -1.769451      18.88
 C       1.484862     1.461529    -0.540206      67.31
 H       1.804710     2.476764    -0.326644      21.97
 C       0.283904     0.978756     0.005585      14.34
 O      -0.501221     1.735503     0.909847     184.00
 C      -0.356386     3.234430     1.129661      81.10
 H      -1.359762     3.614787     1.011866      24.81
 H      -0.129008     3.153391     2.322508      21.42
 H       0.478965     3.673318     0.307169      21.26
 C      -0.237616    -0.251621    -0.408374      21.83
 O      -1.509558    -0.604859     0.014127     141.71
 C       0.537708    -1.210709    -1.099410      46.16
 H       0.184115    -2.367704    -1.374467      20.06
 C       2.402399     0.409792    -1.049338      29.49
 C       3.849404     0.685730    -1.431250     104.57
 H       4.055048     0.321776    -2.315080      25.44
 O       3.930129     2.130800    -1.484951     215.51
 H       4.921219     2.290574    -1.298291      17.36
 C       4.806192     0.098643    -0.399564     102.34
 H       4.941810     0.553694     0.633539      18.29
 O       4.608331    -1.275515    -0.192749     359.02
 H       4.752118    -1.584265    -1.092028      28.28
 C       6.365438     0.365467    -0.877978      92.09
 O       6.686764     1.780613    -0.790117     348.75
 H       6.873395     2.085556     0.185464      29.63
 H       6.575086     0.073109    -1.872905      33.28
 H       6.845593    -0.240597    -0.124118      30.81
55
name= lig-ACN-Water-frame_337
 C      -3.297532     0.690767    -3.321591      66.72
 H      -3.098055    -0.295779    -3.600837      27.12
 C      -4.247549     1.948832    -1.466380      57.18
 H      -4.645417     2.215940    -0.386808      21.63
 C      -4.205067     3.065998    -2.270086      17.45
 O      -4.584547     4.353883    -1.871140     180.43
 C      -4.983722     4.502761    -0.434213     122.77
 H      -4.194166     4.124643     0.107231      26.19
 H      -5.916914     3.945933    -0.237097      26.35
 H      -5.070078     5.677201    -0.093940      24.90
 C      -3.672409     2.956156    -3.678334      17.90
 O      -3.745522     4.105012    -4.477834     180.27
 H      -3.555689     4.969600    -4.003406      23.29
 C      -3.205891     1.805390    -4.138996      73.33
 H      -3.208453     1.698625    -5.252750      23.66
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 C      -3.729903     0.711769    -1.986172      22.42
 C      -3.749763    -0.637070    -1.157507      71.67
 H      -4.435533    -1.333594    -1.695778      24.89
 O      -4.351644    -0.503191     0.231372     189.77
 H      -3.691398    -0.067174     0.900888      22.27
 C      -2.406861    -1.412762    -0.937347      85.59
 H      -1.693369    -1.440046    -1.892136      23.53
 C      -2.567484    -2.800101    -0.374735     106.47
 O      -3.338293    -3.719457    -1.159501     263.69
 H      -2.872622    -4.166256    -1.913142      27.84
 H      -3.225352    -2.871093     0.531444      23.16
 H      -1.485132    -3.344575    -0.392336      21.16
 C       1.838084    -0.869802    -1.412763      39.94
 H       2.483329    -1.606233    -1.873991      18.71
 C       1.573435     1.356965    -0.479112      71.92
 H       2.035308     2.228349    -0.315651      24.38
 C       0.228675     1.087645     0.052379      12.34
 O      -0.506687     1.799359     0.908416     225.45
 C      -0.423526     3.211535     1.080093      98.50
 H      -1.414447     3.654316     0.946495      24.17
 H       0.084541     3.629528     2.215833      21.10
 H       0.356320     3.787194     0.369197      22.44
 C      -0.320208    -0.187995    -0.474910       1.37
 O      -1.611259    -0.644551    -0.084675     209.41
 C       0.533120    -1.118315    -1.103925      49.31
 H       0.025592    -2.153817    -1.533180      19.42
 C       2.317726     0.409984    -1.034249      34.63
 C       3.752551     0.697498    -1.366837     110.44
 H       3.907883     0.232480    -2.205447      25.69
 O       4.044644     2.103916    -1.530870     224.81
 H       4.953467     2.329126    -1.025143      16.18
 C       4.850391     0.088561    -0.406948      86.45
 H       4.540574     0.586903     0.575849      20.71
 O       4.631185    -1.371850    -0.218403     370.62
 H       4.743629    -1.846304    -1.027243      30.59
 C       6.321341     0.375677    -0.841163     110.87
 O       6.681265     1.792561    -0.781098     316.90
 H       6.860327     1.951646     0.260902      28.03
 H       6.435488     0.142929    -1.896922      31.43
 H       7.056457    -0.185014    -0.346329      30.03
55
name= lig-ACN-Water-frame_338
 C      -3.310228     0.564793    -3.329609      40.64
 H      -2.985872    -0.311676    -3.896533      22.89
 C      -4.204191     1.901206    -1.462230      58.82
 H      -4.716470     1.807166    -0.468828      23.30
 C      -4.156939     3.079498    -2.321250      10.46
 O      -4.532817     4.389683    -1.843378     213.21
 C      -4.953482     4.549323    -0.413520     114.48
 H      -4.339918     4.265426     0.375508      26.87
 H      -5.937921     4.114260    -0.164140      26.84
 H      -5.099810     5.740772    -0.501733      25.31
 C      -3.670450     3.030921    -3.582338      15.01
 O      -3.665331     4.059320    -4.454370     187.10
 H      -4.120953     4.748966    -4.062590      28.67
 C      -3.163761     1.769998    -4.172538      32.41
 H      -2.902460     1.743446    -5.248163      24.20
 C      -3.731114     0.663765    -1.948882      10.93
 C      -3.813058    -0.681697    -1.085224      73.80
 H      -4.455892    -1.477245    -1.598951      23.61
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 O      -4.479536    -0.459310     0.201815     221.87
 H      -3.841838     0.179959     0.697236      24.24
 C      -2.411448    -1.421471    -0.996049      62.30
 H      -2.126615    -1.479990    -2.170072      23.41
 C      -2.528186    -2.925209    -0.358975     100.71
 O      -3.325831    -3.759612    -1.232458     261.21
 H      -2.736199    -4.127243    -1.863453      28.71
 H      -2.952405    -2.703941     0.682289      23.58
 H      -1.389062    -3.204272     0.055519      21.90
 C       1.819206    -0.900120    -1.391506      44.41
 H       2.364766    -1.586619    -2.046117      19.65
 C       1.556901     1.357098    -0.237828      48.32
 H       1.986320     2.221357     0.031206      17.62
 C       0.210494     1.034022    -0.052293       7.63
 O      -0.570899     1.840476     0.939379     182.62
 C      -0.433427     3.277160     1.014677      78.97
 H      -1.497392     3.688225     0.947616      22.85
 H       0.022259     3.477767     2.229658      20.02
 H       0.205963     3.643172     0.134768      22.28
 C      -0.390519    -0.164651    -0.436556      19.55
 O      -1.642337    -0.557308    -0.064083     179.77
 C       0.457434    -1.078028    -1.147409      67.73
 H      -0.060352    -2.096620    -1.436076      17.30
 C       2.360339     0.364675    -1.106124      10.54
 C       3.819822     0.672108    -1.433250      92.85
 H       3.986813     0.323410    -2.326747      22.18
 O       4.136742     2.134302    -1.559371     232.67
 H       4.960263     2.282725    -1.002820      16.14
 C       4.831035     0.016047    -0.347224      74.04
 H       4.714576     0.342030     0.708741      21.66
 O       4.672565    -1.434065    -0.244604     406.16
 H       4.802393    -1.731169    -1.223617      27.52
 C       6.280701     0.368796    -0.862178     102.41
 O       6.657032     1.803740    -0.773460     310.98
 H       6.834211     2.042611     0.237504      29.38
 H       6.265195     0.060650    -1.931643      33.80
 H       6.914215    -0.233709    -0.332798      32.01
55
name= lig-ACN-Water-frame_339
 C      -3.286815     0.530373    -3.347104      58.93
 H      -2.931444    -0.479996    -3.697743      23.19
 C      -4.156999     1.838298    -1.502033      54.44
 H      -4.528148     1.919206    -0.522103      20.42
 C      -4.125842     3.075791    -2.158735      40.96
 O      -4.480140     4.350533    -1.779086     214.61
 C      -4.927196     4.636453    -0.485437     127.86
 H      -4.089542     4.373116     0.154282      24.63
 H      -5.859122     4.038401    -0.403847      24.88
 H      -5.096236     5.744645    -0.264097      25.24
 C      -3.624404     2.968231    -3.604673      23.05
 O      -3.591804     4.102853    -4.462009     144.35
 H      -4.264418     4.836250    -4.204986      22.44
 C      -3.276322     1.689706    -4.068732      73.23
 H      -2.585486     1.686548    -4.881854      24.28
 C      -3.750982     0.524031    -2.014632      23.60
 C      -3.905823    -0.705442    -1.057538      83.65
 H      -4.710546    -1.327117    -1.645251      23.53
 O      -4.576022    -0.407686     0.138854     207.16
 H      -4.062782     0.137367     0.759660      24.45
 C      -2.529333    -1.434755    -0.972644      63.05
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 H      -1.867611    -1.484971    -1.981014      21.46
 C      -2.503526    -2.832567    -0.342610      97.42
 O      -3.292602    -3.794607    -1.247720     188.61
 H      -2.812690    -4.107789    -2.089378      26.01
 H      -3.176113    -2.923928     0.579827      22.87
 H      -1.433766    -3.426852    -0.381737      19.71
 C       1.751123    -0.801563    -1.437355      93.53
 H       2.327852    -1.614221    -1.914346      15.09
 C       1.617663     1.226214    -0.181737      46.94
 H       1.975476     2.045791     0.397580      14.05
 C       0.153443     1.078270     0.051310       6.11
 O      -0.621251     1.783152     0.888141     221.18
 C      -0.451878     3.297623     0.934907      71.47
 H      -1.507636     3.796691     1.007146      20.60
 H       0.294565     3.655676     2.000454      18.71
 H       0.208988     3.675976     0.177357      23.06
 C      -0.347619    -0.218019    -0.437285       5.89
 O      -1.695436    -0.465829    -0.069639     137.93
 C       0.380310    -1.141916    -1.149543      55.48
 H       0.036200    -2.140185    -1.456585      18.59
 C       2.390839     0.458465    -1.022448      40.50
 C       3.923130     0.685263    -1.446509      79.33
 H       4.161296     0.187484    -2.258555      24.53
 O       4.141112     2.124512    -1.545569     260.93
 H       5.033114     2.278609    -1.269051      18.99
 C       4.805915    -0.029690    -0.358877      89.41
 H       4.676873     0.411638     0.616108      22.22
 O       4.721401    -1.461504    -0.314716     410.25
 H       4.856249    -1.862388    -1.308444      24.88
 C       6.267372     0.328645    -0.863690     115.03
 O       6.597689     1.770444    -0.775701     327.05
 H       6.988645     1.881253     0.156433      31.72
 H       6.481914     0.182066    -1.966858      33.68
 H       6.985715    -0.194052    -0.341671      30.66
55
name= lig-ACN-Water-frame_340
 C      -3.290016     0.427974    -3.282092      49.92
 H      -2.809962    -0.450734    -3.818409      20.42
 C      -4.144398     1.781978    -1.439079      65.16
 H      -4.353116     1.803381    -0.464023      23.59
 C      -4.019546     2.995606    -2.235910      24.01
 O      -4.397159     4.332370    -1.823276     222.95
 C      -4.871117     4.622753    -0.458120     121.22
 H      -4.210650     4.304417     0.375162      27.53
 H      -5.789970     4.134937    -0.043675      27.94
 H      -5.022161     5.729418    -0.483635      28.41
 C      -3.695293     2.961851    -3.546655      18.06
 O      -3.515904     4.057296    -4.444387     107.48
 H      -3.751900     4.963965    -3.849379      18.34
 C      -3.268194     1.705378    -4.053863      54.12
 H      -3.087987     1.686204    -5.118519      25.25
 C      -3.843531     0.547651    -1.994957      34.23
 C      -3.985708    -0.706350    -1.193213      62.11
 H      -4.541759    -1.664792    -1.637677      22.35
 O      -4.682916    -0.374191     0.136993     183.77
 H      -3.946204    -0.060134     0.677134      26.18
 C      -2.574365    -1.351867    -0.847536      75.37
 H      -2.165368    -1.388274    -1.987416      23.41
 C      -2.587927    -2.854405    -0.438393     114.44
 O      -3.280033    -3.786975    -1.220729     239.07
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 H      -2.748958    -3.947176    -2.130136      24.24
 H      -2.857226    -2.945146     0.663524      24.98
 H      -1.350241    -2.951014    -0.253859      22.13
 C       1.728967    -0.697890    -1.503047      29.02
 H       2.402199    -1.342629    -2.102098      17.66
 C       1.596305     1.245618    -0.083111      59.57
 H       2.259992     2.031878     0.385833      20.62
 C       0.269406     0.902980     0.119037      12.60
 O      -0.672720     1.837542     0.836474     155.43
 C      -0.404757     3.215927     0.867784      95.58
 H      -1.509199     3.697022     0.957053      22.83
 H       0.223574     3.521459     2.018572      20.99
 H       0.013471     3.527236    -0.037019      26.11
 C      -0.420509    -0.229617    -0.401873       0.50
 O      -1.789426    -0.441777    -0.124771     169.47
 C       0.479105    -1.148487    -1.116817      65.17
 H       0.108259    -2.020188    -1.458922      22.38
 C       2.375020     0.391430    -1.003058      31.99
 C       3.820274     0.674864    -1.358196      94.20
 H       3.836921     0.342728    -2.289003      23.77
 O       4.108855     2.086967    -1.526110     231.30
 H       5.024887     2.227660    -1.283864      19.38
 C       4.916582     0.001535    -0.452595     109.01
 H       4.632874     0.231252     0.532798      22.44
 O       4.731321    -1.478986    -0.384268     399.80
 H       4.951654    -1.867504    -1.363293      24.32
 C       6.349248     0.287296    -0.839359      90.30
 O       6.562000     1.731013    -0.762621     310.63
 H       6.724069     1.931630     0.178651      31.41
 H       6.337871    -0.145204    -1.894045      32.11
 H       7.065140    -0.289455    -0.273930      31.49
55
name= lig-ACN-Water-frame_341
 C      -3.348229     0.549556    -3.328029      59.12
 H      -3.163691    -0.474970    -3.727120      22.94
 C      -4.143611     1.851884    -1.381170      54.36
 H      -4.561368     1.909098    -0.434065      21.02
 C      -4.036900     2.989905    -2.179839      39.98
 O      -4.315519     4.264063    -1.813107     202.00
 C      -4.784001     4.584545    -0.425743     117.74
 H      -3.931200     4.460944     0.349675      24.57
 H      -5.761068     4.068862    -0.449565      24.94
 H      -4.919863     5.598097    -0.457362      29.08
 C      -3.633834     2.889418    -3.606553      22.76
 O      -3.479470     3.982806    -4.359567     131.24
 H      -3.493832     4.893845    -4.004358      20.43
 C      -3.267106     1.624121    -4.137566      65.85
 H      -3.185867     1.497178    -5.212830      25.74
 C      -3.894893     0.530744    -2.006272      16.51
 C      -4.039577    -0.719797    -1.075119      94.11
 H      -4.718092    -1.436164    -1.782603      23.56
 O      -4.759733    -0.414393     0.070231     218.62
 H      -4.189774    -0.046202     0.831471      23.05
 C      -2.665013    -1.295913    -0.992315      71.76
 H      -2.133883    -1.407941    -2.036096      22.28
 C      -2.553012    -2.801454    -0.351840      98.54
 O      -3.294760    -3.755193    -1.230641     244.17
 H      -2.765425    -4.039230    -2.003315      28.87
 H      -3.101331    -2.895986     0.624286      23.53
 H      -1.427085    -3.270396    -0.473524      20.37
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 C       1.781446    -0.740623    -1.553389      48.78
 H       2.170128    -1.327019    -2.402484      19.94
 C       1.627097     1.220987    -0.024760      58.94
 H       1.864165     2.288958     0.403636      18.05
 C       0.218020     0.886093     0.261441       5.15
 O      -0.677694     1.745046     0.752949     192.20
 C      -0.387920     3.167228     0.804505      94.64
 H      -1.407275     3.752405     1.054819      22.24
 H       0.556588     3.501199     1.720002      20.27
 H       0.156468     3.509646    -0.020112      25.16
 C      -0.389013    -0.310322    -0.354589       2.72
 O      -1.794582    -0.406838    -0.131687     158.70
 C       0.434964    -1.122365    -1.102116      65.75
 H       0.122381    -1.932341    -1.537243      23.00
 C       2.340348     0.430887    -0.891721      36.40
 C       3.751918     0.660871    -1.391110      90.27
 H       3.894603     0.167063    -2.248494      25.37
 O       4.033044     2.096340    -1.489196     201.36
 H       4.919426     2.176538    -0.985592      16.90
 C       4.897859    -0.098199    -0.428395      90.56
 H       4.943670     0.323791     0.519560      21.04
 O       4.726843    -1.468563    -0.448317     321.72
 H       4.980668    -1.751848    -1.429265      25.35
 C       6.400339     0.233598    -0.851275     102.62
 O       6.584492     1.700846    -0.745610     290.24
 H       6.766360     1.939450     0.170917      32.36
 H       6.841361     0.145066    -1.879227      29.04
 H       7.031975    -0.280810    -0.062521      29.14
55
name= lig-ACN-Water-frame_342
 C      -3.514852     0.476789    -3.319525      51.02
 H      -3.418531    -0.506508    -3.747961      24.82
 C      -4.188467     1.842281    -1.400684      63.64
 H      -4.604351     1.964307    -0.376282      20.46
 C      -4.026304     2.952022    -2.223736      23.27
 O      -4.223117     4.298412    -1.768402     260.94
 C      -4.694801     4.541109    -0.494235     129.24
 H      -3.954822     3.998590     0.279742      23.57
 H      -5.537659     3.961840    -0.063563      25.81
 H      -4.901753     5.494601    -0.353664      27.77
 C      -3.525091     2.818659    -3.550921      45.43
 O      -3.437249     3.974041    -4.374507     240.59
 H      -3.911394     4.596392    -3.901184      28.55
 C      -3.338359     1.620049    -4.226524      50.36
 H      -2.740204     1.594838    -5.160048      18.84
 C      -3.897012     0.652429    -1.936649      40.78
 C      -4.066788    -0.639951    -1.146583      70.68
 H      -4.768981    -1.517525    -1.633437      21.48
 O      -4.858997    -0.485229     0.104263     184.84
 H      -4.276610     0.059703     0.756221      23.52
 C      -2.574870    -1.417615    -1.022668      58.59
 H      -2.230054    -1.295328    -2.079117      24.31
 C      -2.572687    -2.746145    -0.392974     111.50
 O      -3.344787    -3.702943    -1.237331     250.38
 H      -2.754922    -4.091711    -1.851222      29.73
 H      -3.068805    -2.657019     0.603995      25.13
 H      -1.444734    -2.997816    -0.020400      23.46
 C       1.690812    -0.738064    -1.416161       2.57
 H       2.365530    -1.305777    -2.079942      19.52
 C       1.513261     1.164907     0.051937      62.76
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 H       2.084962     2.150668     0.311691      18.89
 C       0.229528     0.834642     0.248385      18.65
 O      -0.759181     1.736986     0.754950     193.28
 C      -0.304036     3.130874     0.760207      85.29
 H      -1.280779     3.702624     1.090204      22.66
 H       0.527487     3.229015     1.802057      20.50
 H      -0.014871     3.465397    -0.230683      25.46
 C      -0.346673    -0.347650    -0.256207       4.88
 O      -1.752558    -0.401325    -0.163059     100.25
 C       0.395221    -1.159194    -1.198445      66.23
 H      -0.085467    -1.899682    -1.678878      21.15
 C       2.357018     0.349128    -0.919207      44.92
 C       3.831176     0.656970    -1.353703     104.00
 H       3.896544     0.381963    -2.335611      26.72
 O       3.968872     2.116048    -1.442911     188.88
 H       4.842694     2.359083    -0.937516      22.32
 C       4.914869    -0.061854    -0.467027      99.56
 H       4.601722     0.105596     0.513703      26.08
 O       4.692829    -1.528929    -0.478578     386.32
 H       4.848015    -1.934186    -1.405726      28.47
 C       6.390066     0.264218    -0.831978      93.43
 O       6.634011     1.705447    -0.674048     201.57
 H       6.958814     1.775041     0.297639      26.45
 H       6.467404    -0.153560    -1.851065      32.54
 H       7.156888    -0.346957    -0.156566      30.42
55
name= lig-ACN-Water-frame_343
 C      -3.668447     0.409625    -3.367379      60.72
 H      -3.466845    -0.554670    -3.738664      21.86
 C      -4.253306     1.910434    -1.406064      48.54
 H      -4.500247     1.951223    -0.255493      20.51
 C      -3.971953     3.028140    -2.256997       3.43
 O      -4.142712     4.316738    -1.854519     207.12
 C      -4.617268     4.427749    -0.390105     108.75
 H      -3.715309     4.253608     0.391563      24.13
 H      -5.596507     3.994470    -0.446788      27.44
 H      -4.633035     5.421320    -0.302435      27.83
 C      -3.514746     2.888358    -3.586526       8.93
 O      -3.394180     3.977914    -4.359642     186.78
 H      -3.952206     4.830075    -4.114799      23.41
 C      -3.343662     1.537564    -4.093299      73.54
 H      -3.058929     1.453882    -5.187000      28.33
 C      -3.940173     0.571273    -1.979130      22.77
 C      -4.031775    -0.685828    -1.167796      63.81
 H      -4.600492    -1.415329    -1.977766      20.69
 O      -4.860598    -0.528103     0.131521     168.88
 H      -4.388403     0.040760     0.774700      24.89
 C      -2.545127    -1.277162    -1.011668      84.37
 H      -2.065995    -1.508795    -1.946754      24.42
 C      -2.662191    -2.736699    -0.370882     105.51
 O      -3.350692    -3.645542    -1.212242     199.01
 H      -2.746236    -4.061592    -1.950900      25.54
 H      -3.302079    -2.682011     0.536566      24.43
 H      -1.588741    -3.220460    -0.222760      22.91
 C       1.725539    -0.862763    -1.397211      41.00
 H       2.263762    -1.621833    -1.977735      17.50
 C       1.617242     1.124474     0.000354      51.75
 H       1.985384     2.028359     0.507535      17.34
 C       0.158452     0.817492     0.240747     -18.10
 O      -0.794752     1.746258     0.775221     184.62
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 C      -0.310426     3.075651     0.787516      91.90
 H      -1.131378     3.789243     1.132527      23.07
 H       0.805426     3.354056     1.491014      19.90
 H       0.178192     3.324505    -0.202255      23.82
 C      -0.414707    -0.413995    -0.306643      18.79
 O      -1.765012    -0.476685    -0.204306     183.09
 C       0.323887    -1.162950    -1.191599      78.23
 H      -0.031419    -1.981634    -1.825776      20.78
 C       2.346992     0.311787    -0.834215      36.70
 C       3.807138     0.671783    -1.341114      84.49
 H       3.932023     0.242382    -2.313196      23.97
 O       3.955003     2.166359    -1.368531     202.68
 H       4.751591     2.381077    -0.871531      20.79
 C       4.857116    -0.086666    -0.419920      94.33
 H       4.772705     0.269087     0.592554      24.04
 O       4.657287    -1.569134    -0.502785     352.42
 H       4.914438    -1.695338    -1.445519      27.99
 C       6.293983     0.287819    -0.792089      98.21
 O       6.693250     1.690397    -0.592633     262.65
 H       6.906099     1.931618     0.425205      27.65
 H       6.440362     0.325601    -1.877260      30.44
 H       7.091718    -0.490112    -0.302994      28.55
55
name= lig-ACN-Water-frame_344
 C      -3.719839     0.405681    -3.340037      51.61
 H      -3.689869    -0.557641    -3.803267      20.69
 C      -4.183090     1.857341    -1.535121      59.72
 H      -4.480631     2.042699    -0.407641      19.50
 C      -3.932608     3.016942    -2.212699      25.95
 O      -4.092378     4.369030    -1.804347     269.93
 C      -4.504932     4.468542    -0.442316     119.94
 H      -3.864566     3.685314     0.266127      24.08
 H      -5.392588     3.927845    -0.226276      28.57
 H      -4.739928     5.425879    -0.128997      27.38
 C      -3.587081     2.851658    -3.598026      14.48
 O      -3.319799     4.018649    -4.443941     126.25
 H      -3.505453     4.841016    -3.755553      20.92
 C      -3.371550     1.573350    -4.078845      71.54
 H      -3.399079     1.411387    -5.189314      28.09
 C      -4.106358     0.567613    -1.981858      38.44
 C      -4.015915    -0.704384    -1.112577      92.40
 H      -4.636505    -1.685613    -1.508800      21.07
 O      -4.760650    -0.592633     0.049819     234.76
 H      -4.259057    -0.138495     0.740506      25.04
 C      -2.641448    -1.333548    -1.009913      83.63
 H      -2.301045    -1.228286    -1.986033      26.53
 C      -2.734315    -2.715378    -0.327764     110.41
 O      -3.413304    -3.653890    -1.253356     204.42
 H      -2.768609    -3.801454    -2.039938      26.46
 H      -3.253573    -2.697124     0.642751      24.82
 H      -1.634055    -3.014785    -0.041065      24.09
 C       1.767834    -0.980530    -1.385051       3.26
 H       2.312890    -1.563477    -2.127336      18.97
 C       1.497037     1.091903     0.023988      59.54
 H       1.976235     1.934976     0.366216      20.61
 C       0.163666     0.820146     0.211688      18.52
 O      -0.729892     1.677821     0.797433     195.67
 C      -0.265539     3.111831     0.794254      85.67
 H      -1.114472     3.684464     1.178595      24.13
 H       0.640941     3.090754     1.747322      19.83
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 H      -0.014694     3.491579    -0.301799      23.41
 C      -0.443584    -0.314656    -0.417370       1.47
 O      -1.838741    -0.471731    -0.125621     160.54
 C       0.403796    -1.209518    -1.180800      54.75
 H      -0.136489    -2.159464    -1.618323      18.69
 C       2.351074     0.186349    -0.859006      33.49
 C       3.709974     0.667242    -1.253619      85.74
 H       3.947906     0.379040    -2.286800      21.08
 O       3.957887     2.155021    -1.285409     248.97
 H       4.808872     2.255310    -0.851874      19.38
 C       4.797146    -0.086545    -0.342052      84.28
 H       4.594277     0.025686     0.753442      21.48
 O       4.648959    -1.497738    -0.537853     373.70
 H       4.893474    -1.869300    -1.407582      31.85
 C       6.268700     0.332921    -0.855293      82.59
 O       6.686125     1.682292    -0.476956     300.75
 H       7.092376     1.630977     0.546343      24.42
 H       6.356889     0.093256    -1.921166      31.23
 H       6.985704    -0.462851    -0.257464      27.01
55
name= lig-ACN-Water-frame_345
 C      -3.749597     0.446232    -3.359981      58.19
 H      -3.778196    -0.521297    -3.910718      26.85
 C      -4.157354     1.828134    -1.449639      51.22
 H      -4.491016     1.870079    -0.352100      19.40
 C      -3.912280     3.049078    -2.306209      10.60
 O      -4.031735     4.375707    -1.758060     236.44
 C      -4.474448     4.442387    -0.396697     107.60
 H      -3.538671     4.078333     0.319452      21.80
 H      -5.443744     4.086043    -0.377214      26.10
 H      -4.255356     5.508375    -0.175848      24.35
 C      -3.565553     2.932075    -3.653842      31.78
 O      -3.275723     3.981625    -4.435702     247.60
 H      -3.023299     4.743459    -3.937898      29.51
 C      -3.530627     1.591736    -4.213080      61.60
 H      -3.012834     1.549372    -5.205065      18.86
 C      -4.149644     0.503095    -2.040168      38.43
 C      -4.137623    -0.749153    -1.184390      88.10
 H      -4.674028    -1.492422    -1.974812      22.87
 O      -4.715162    -0.634601     0.140077     203.23
 H      -4.080210    -0.127516     0.770230      21.45
 C      -2.709748    -1.350955    -0.967467      81.09
 H      -2.212917    -1.578086    -1.831543      28.33
 C      -2.768818    -2.739544    -0.347560     110.64
 O      -3.454217    -3.668755    -1.274066     212.83
 H      -2.957405    -3.819795    -2.040464      31.26
 H      -3.459826    -2.679966     0.528600      24.54
 H      -1.732936    -3.100502    -0.086937      24.84
 C       1.775763    -1.004983    -1.388851      55.38
 H       2.399429    -1.622591    -2.036934      18.86
 C       1.499943     0.998664    -0.041724      79.45
 H       1.962356     1.855177     0.236009      21.97
 C       0.132836     0.797827     0.104187       8.93
 O      -0.668815     1.704161     0.839895     180.09
 C      -0.302087     3.071002     0.888869      98.18
 H      -1.186577     3.574541     1.245847      23.82
 H       0.725293     3.450468     1.650711      20.99
 H       0.168179     3.473373    -0.176969      23.09
 C      -0.469639    -0.297700    -0.506510       2.92
 O      -1.822505    -0.443406    -0.073351     151.71
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 C       0.369026    -1.280512    -1.108816      77.21
 H      -0.072401    -2.352046    -1.517930      21.65
 C       2.255587     0.190882    -0.851067      28.69
 C       3.729512     0.655864    -1.163663      85.27
 H       3.768368     0.257489    -2.227814      22.85
 O       3.922311     2.089729    -1.166159     230.31
 H       4.860527     2.343353    -0.824903      17.53
 C       4.802895    -0.049805    -0.388809      99.10
 H       4.662082     0.206394     0.726349      23.27
 O       4.640143    -1.479640    -0.551453     367.98
 H       5.007460    -1.584001    -1.502862      28.41
 C       6.222733     0.308630    -0.763250      90.29
 O       6.630696     1.649282    -0.444820     279.12
 H       7.051528     1.761948     0.539415      24.53
 H       6.229627     0.358467    -1.876949      30.30
 H       7.055030    -0.500235    -0.389278      28.00
55
name= lig-ACN-Water-frame_346
 C      -3.846160     0.503752    -3.539421      37.12
 H      -3.561708    -0.541820    -3.936815      21.62
 C      -4.162817     1.887308    -1.458285      45.42
 H      -4.334000     2.037472    -0.412364      20.10
 C      -3.964359     2.982565    -2.219106      58.75
 O      -3.940790     4.288290    -1.793489     218.53
 C      -4.354419     4.517846    -0.312256     108.84
 H      -3.887607     3.800403     0.538100      22.73
 H      -5.343700     4.233472    -0.142786      26.67
 H      -4.516954     5.667109    -0.198595      22.88
 C      -3.556188     2.877624    -3.645542      45.21
 O      -3.200859     3.989768    -4.476328     235.06
 H      -3.106786     4.764247    -3.925859      32.84
 C      -3.605303     1.641709    -4.275793      52.32
 H      -3.218484     1.433821    -5.286728      20.39
 C      -4.059726     0.605649    -2.071406      39.94
 C      -4.161960    -0.761585    -1.258919      52.99
 H      -4.913301    -1.596961    -1.519181      20.83
 O      -4.771808    -0.696913     0.203929     114.82
 H      -4.259567     0.024052     0.782117      22.04
 C      -2.655913    -1.354294    -0.984734      73.35
 H      -2.196829    -1.313317    -1.894460      26.65
 C      -2.858308    -2.828015    -0.337837     110.79
 O      -3.504392    -3.682057    -1.294290     210.11
 H      -2.844574    -3.980411    -1.994025      26.87
 H      -3.493599    -2.865837     0.588922      24.35
 H      -1.875470    -3.231407    -0.086838      25.22
 C       1.660587    -1.005026    -1.368405      30.69
 H       2.225751    -1.857751    -1.753470      16.85
 C       1.520122     1.059905    -0.097024      45.89
 H       1.856061     1.893658     0.509268      18.47
 C       0.093432     0.868827     0.038925      -5.46
 O      -0.634653     1.680175     0.883432     195.92
 C      -0.304104     3.105691     0.975084      80.80
 H      -1.195752     3.652321     1.266423      22.34
 H       0.629601     3.191924     1.898856      19.37
 H      -0.055388     3.527099    -0.181049      20.85
 C      -0.529013    -0.393609    -0.464471       5.47
 O      -1.861626    -0.499868    -0.151113     175.16
 C       0.334849    -1.344046    -1.095577      56.28
 H      -0.069880    -2.449609    -1.474429      20.73
 C       2.325368     0.190978    -0.885063      40.80
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 C       3.716819     0.612452    -1.215680      86.56
 H       4.106184     0.405468    -2.246302      21.68
 O       3.848349     2.065231    -1.042571     219.34
 H       4.780743     2.143910    -0.616259      17.29
 C       4.809525    -0.084601    -0.324704      91.46
 H       4.671255     0.147436     0.822167      21.42
 O       4.652550    -1.492739    -0.568497     373.03
 H       5.025504    -1.869753    -1.468102      25.87
 C       6.234195     0.303768    -0.759480      91.32
 O       6.578251     1.678805    -0.425597     288.28
 H       6.736179     1.791880     0.552138      29.84
 H       6.363931     0.154770    -1.879382      30.69
 H       6.942702    -0.557017    -0.299067      29.34
55
name= lig-ACN-Water-frame_347
 C      -3.920645     0.489971    -3.494090      82.56
 H      -3.932359    -0.543945    -4.067836      19.90
 C      -4.172960     1.798684    -1.483861      44.10
 H      -4.341003     1.851274    -0.471768      19.85
 C      -3.916074     3.033430    -2.302365     -14.91
 O      -3.871799     4.274876    -1.666780     258.69
 C      -4.324690     4.556142    -0.365534      84.00
 H      -3.471181     4.134433     0.313378      24.24
 H      -5.319572     4.186683    -0.258527      26.52
 H      -3.995863     5.703058    -0.114715      22.07
 C      -3.585646     2.899016    -3.660164      26.63
 O      -3.149068     3.974398    -4.427346     161.29
 H      -3.558707     4.886897    -3.999375      22.88
 C      -3.592760     1.670984    -4.328752      70.95
 H      -3.698818     1.826885    -5.396336      30.39
 C      -4.046899     0.570393    -2.111562      34.77
 C      -4.093345    -0.692933    -1.108049      92.81
 H      -4.550598    -1.367168    -1.873962      22.96
 O      -4.839909    -0.715309     0.109671     218.42
 H      -4.407459    -0.059089     0.784623      22.76
 C      -2.744077    -1.446812    -1.070381      76.33
 H      -2.351983    -1.658573    -1.998580      25.81
 C      -2.858208    -2.865722    -0.368585     112.88
 O      -3.560741    -3.723160    -1.351807     171.53
 H      -2.834574    -4.165609    -1.981124      24.62
 H      -3.529731    -2.607324     0.503241      24.07
 H      -1.906484    -3.210485    -0.056608      24.92
 C       1.653909    -1.028965    -1.318015      34.41
 H       2.308595    -1.696019    -1.909315      20.31
 C       1.444579     1.123876    -0.160381      46.36
 H       2.124579     1.974803     0.288996      17.43
 C       0.135177     0.838668     0.027772      17.30
 O      -0.682672     1.647055     0.907440     180.25
 C      -0.321233     3.099115     1.040685      87.21
 H      -1.252031     3.536808     1.528727      21.91
 H       0.657642     3.307455     1.871103      21.82
 H       0.187119     3.678735     0.030442      20.76
 C      -0.514666    -0.372166    -0.367896       9.66
 O      -1.939121    -0.557196    -0.208373     140.92
 C       0.252243    -1.326668    -1.073037      74.94
 H      -0.188615    -2.391875    -1.390549      18.47
 C       2.253379     0.165527    -0.936323      23.66
 C       3.788815     0.601786    -1.229344      85.98
 H       3.903617     0.383927    -2.359978      20.55
 O       3.790010     2.050810    -0.927164     242.72
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 H       4.638801     2.326203    -0.586551      21.23
 C       4.806656    -0.176836    -0.359100      86.37
 H       4.509617    -0.074217     0.780131      22.09
 O       4.668723    -1.592886    -0.534899     389.15
 H       5.091675    -1.705163    -1.462190      26.52
 C       6.274990     0.277220    -0.727173      98.37
 O       6.525546     1.724833    -0.412403     277.73
 H       6.887741     1.736856     0.456550      30.40
 H       6.432006     0.067739    -1.859090      30.76
 H       7.075715    -0.233314    -0.076603      27.82
55
name= lig-ACN-Water-frame_348
 C      -3.914011     0.468291    -3.523755      50.12
 H      -4.371912    -0.442775    -4.074398      27.14
 C      -4.131927     1.863945    -1.554079      32.75
 H      -4.329462     1.939732    -0.532053      18.80
 C      -3.877101     2.999548    -2.222112      58.49
 O      -3.771098     4.313136    -1.705982     242.73
 C      -4.207385     4.543672    -0.336550     108.41
 H      -3.686432     4.012568     0.513325      26.22
 H      -5.275280     4.315418    -0.122656      26.94
 H      -4.427191     5.756933    -0.359006      22.58
 C      -3.595121     2.954731    -3.647765      41.39
 O      -3.135374     4.034249    -4.351664      88.21
 H      -3.710040     4.925226    -4.215855      20.21
 C      -3.694411     1.634372    -4.241851      45.97
 H      -3.482944     1.412404    -5.294078      19.09
 C      -4.067429     0.493567    -2.054307      48.81
 C      -4.112130    -0.752186    -1.253849      87.78
 H      -4.812130    -1.457768    -1.711603      22.43
 O      -4.882545    -0.655412    -0.004260     205.17
 H      -4.335437    -0.286458     0.711950      24.65
 C      -2.761270    -1.498487    -1.081158      76.33
 H      -2.355688    -1.488429    -2.070304      25.05
 C      -2.908757    -2.850895    -0.447667     115.59
 O      -3.561432    -3.781663    -1.380153     207.01
 H      -2.979821    -4.194431    -2.023168      28.70
 H      -3.627308    -2.958130     0.404776      23.69
 H      -1.899607    -3.211771    -0.185268      24.80
 C       1.650444    -1.074938    -1.327415      47.28
 H       2.116165    -1.832574    -1.996199      19.70
 C       1.451844     1.088781    -0.264784      43.94
 H       1.749848     2.241187    -0.006003      18.62
 C       0.044775     0.828037     0.181560       0.48
 O      -0.724091     1.681854     0.881619     191.74
 C      -0.313431     3.017847     1.142981      86.95
 H      -1.266341     3.657920     1.453416      20.38
 H       0.630582     3.049074     2.002963      20.25
 H      -0.107074     3.488942    -0.025098      20.68
 C      -0.562454    -0.394976    -0.374276      11.16
 O      -1.899647    -0.563068    -0.226476     166.45
 C       0.285300    -1.274630    -1.036342      54.65
 H      -0.197363    -2.184749    -1.469233      21.96
 C       2.221186     0.210213    -0.942116      47.59
 C       3.668402     0.600247    -1.182980      99.35
 H       4.039187     0.517921    -2.295602      21.98
 O       3.782566     2.017983    -0.852229     211.46
 H       4.709712     2.176356    -0.671590      19.16
 C       4.828506    -0.240402    -0.403448      77.91
 H       4.649906     0.119860     0.711466      22.90
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 O       4.718516    -1.712734    -0.538175     343.39
 H       4.989861    -2.022165    -1.433806      29.09
 C       6.302205     0.277368    -0.596027      97.98
 O       6.477106     1.737116    -0.420980     266.27
 H       6.861213     1.987712     0.471422      28.33
 H       6.602442     0.250674    -1.719374      28.92
 H       6.988653    -0.437064    -0.096508      29.34
55
name= lig-ACN-Water-frame_349
 C      -3.989477     0.441066    -3.458795      60.93
 H      -3.907329    -0.518715    -4.022518      24.40
 C      -4.083555     1.804649    -1.439311      65.91
 H      -4.243995     1.924927    -0.355799      17.54
 C      -3.806834     3.052321    -2.238335      51.51
 O      -3.681469     4.313915    -1.740290     163.64
 C      -4.215439     4.562710    -0.303474      75.40
 H      -3.462503     4.197789     0.349583      28.05
 H      -5.158339     3.924039    -0.324065      26.13
 H      -4.134085     5.719640    -0.037981      22.95
 C      -3.599419     2.889533    -3.614321      36.05
 O      -3.146392     4.106187    -4.330537     114.52
 H      -3.528580     4.856773    -3.890733      26.66
 C      -3.733598     1.656441    -4.187521      76.10
 H      -3.389171     1.665261    -5.233315      18.53
 C      -4.098062     0.568746    -2.126344      29.44
 C      -4.271863    -0.858318    -1.379258      68.65
 H      -4.683626    -1.617906    -1.988181      24.43
 O      -4.896302    -0.566315    -0.073306     196.88
 H      -4.183742    -0.234255     0.480129      25.17
 C      -2.719038    -1.388785    -1.110451      68.94
 H      -2.134262    -1.555868    -2.044715      25.49
 C      -2.938289    -2.950498    -0.507577     109.03
 O      -3.542189    -3.849221    -1.445935     220.83
 H      -2.899904    -4.004509    -2.134062      28.75
 H      -3.479163    -2.743652     0.432574      24.65
 H      -1.906595    -3.327373    -0.191690      24.64
 C       1.656381    -1.029015    -1.348341      38.43
 H       2.288444    -1.848421    -1.766856      19.95
 C       1.253168     1.103414    -0.238904      34.06
 H       1.768707     2.166594    -0.081324      20.50
 C       0.053129     0.759866     0.188331      29.16
 O      -0.841717     1.671936     0.881915     183.02
 C      -0.312897     2.980689     1.168399      95.11
 H      -1.202426     3.551034     1.782039      21.31
 H       0.677595     2.936216     1.936285      22.98
 H       0.230927     3.652834     0.231999      22.87
 C      -0.535974    -0.370250    -0.365043       2.97
 O      -1.945916    -0.582420    -0.208083     150.32
 C       0.312114    -1.309864    -1.070907      62.12
 H      -0.096829    -2.153518    -1.501653      24.37
 C       2.219418     0.141460    -0.945362      11.42
 C       3.669694     0.579932    -1.199277      89.83
 H       3.774054     0.403668    -2.380860      21.47
 O       3.811179     1.977450    -0.807897     164.02
 H       4.817629     2.152686    -0.595898      15.80
 C       4.791069    -0.265843    -0.353981      86.32
 H       4.500048    -0.328483     0.764370      22.27
 O       4.767264    -1.738601    -0.511897     371.14
 H       5.184823    -1.841702    -1.395740      27.51
 C       6.294209     0.254952    -0.607036      95.80
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 O       6.455129     1.727659    -0.378408     215.28
 H       6.677092     1.698148     0.665668      24.26
 H       6.644151    -0.124215    -1.636132      29.63
 H       6.890307    -0.128401     0.170908      29.71
55
name= lig-ACN-Water-frame_350
 C      -3.998764     0.526954    -3.537418      43.48
 H      -3.759509    -0.441872    -3.891016      20.71
 C      -4.014742     1.830571    -1.396775      40.06
 H      -4.095862     1.786559    -0.254371      18.54
 C      -3.770460     2.964051    -2.128958       9.77
 O      -3.632052     4.364755    -1.658622     281.50
 C      -4.119716     4.487761    -0.379273     103.25
 H      -3.483835     4.109479     0.333993      30.16
 H      -5.186541     4.025781    -0.097761      24.78
 H      -4.489053     5.558956    -0.276583      22.74
 C      -3.555945     2.975325    -3.580605       4.73
 O      -3.222767     4.037108    -4.280926     152.48
 H      -3.240356     4.799414    -3.749504      23.58
 C      -3.663737     1.685931    -4.296069      82.93
 H      -3.720587     1.607219    -5.397603      31.43
 C      -4.217333     0.540806    -2.084580      33.08
 C      -4.188585    -0.731252    -1.373352      92.70
 H      -4.830053    -1.359906    -1.839655      25.88
 O      -4.913339    -0.561156    -0.153932     174.89
 H      -4.355399     0.008022     0.512806      24.94
 C      -2.784379    -1.476673    -1.155330      65.34
 H      -2.245538    -1.359709    -2.184051      24.48
 C      -2.856208    -2.888287    -0.558100     103.83
 O      -3.520891    -3.870541    -1.520877     158.77
 H      -2.926166    -4.215776    -2.329233      24.25
 H      -3.652880    -3.018870     0.189334      23.79
 H      -1.842913    -3.370482    -0.213036      23.40
 C       1.668407    -1.059701    -1.335085      36.15
 H       2.391618    -1.743485    -1.838314      17.42
 C       1.361782     1.106542    -0.235988      59.04
 H       1.777718     2.025513     0.223237      20.42
 C      -0.088999     0.792661     0.147273      -8.13
 O      -0.895068     1.627805     0.828481     165.69
 C      -0.253116     2.953744     1.255790      74.92
 H      -1.109726     3.621294     1.767096      21.20
 H       0.647181     2.658489     2.012008      21.79
 H      -0.020854     3.538692     0.150033      20.61
 C      -0.584200    -0.496874    -0.399481       9.06
 O      -1.998839    -0.593187    -0.171148     135.42
 C       0.247687    -1.369426    -1.130688      64.25
 H      -0.093250    -2.278228    -1.351278      24.45
 C       2.145507     0.236899    -0.858657      41.78
 C       3.701365     0.517070    -1.154995      84.75
 H       4.042330     0.372977    -2.304805      21.56
 O       3.847943     1.935191    -0.827683     163.56
 H       4.784653     2.090164    -0.367133      15.08
 C       4.732152    -0.312110    -0.298819      95.10
 H       4.464900     0.116908     0.722012      22.99
 O       4.810429    -1.698876    -0.501218     376.03
 H       5.240609    -1.957210    -1.338163      28.30
 C       6.209002     0.202658    -0.499290     110.30
 O       6.430675     1.661514    -0.334908     299.97
 H       6.903187     1.886086     0.562978      29.23
 H       6.599973     0.104711    -1.561472      30.03
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 H       6.822311    -0.394843     0.081011      31.55
55
name= lig-ACN-Water-frame_351
 C      -3.948901     0.623633    -3.560696      75.01
 H      -4.361522    -0.144742    -4.098866      26.88
 C      -3.998312     1.807547    -1.427071      64.94
 H      -4.000347     1.927650    -0.285185      16.22
 C      -3.673933     3.004782    -2.131693      32.34
 O      -3.587221     4.246830    -1.654730     200.47
 C      -4.126033     4.504283    -0.281446      90.33
 H      -3.489750     4.302750     0.469412      31.89
 H      -5.069140     3.775074    -0.359619      25.78
 H      -4.273260     5.536400    -0.209441      24.54
 C      -3.544839     2.854465    -3.533860      36.08
 O      -3.285863     4.037498    -4.271486     166.40
 H      -3.311186     4.924447    -3.686593      21.12
 C      -3.648326     1.747297    -4.276780      46.22
 H      -3.466297     1.763724    -5.367878      20.28
 C      -4.141348     0.669463    -2.170893      36.40
 C      -4.159042    -0.698036    -1.322042      70.92
 H      -4.608624    -1.388482    -1.903818      27.44
 O      -4.948882    -0.588302    -0.106749     166.76
 H      -4.585433     0.050530     0.577400      24.02
 C      -2.822997    -1.445926    -1.166107      66.79
 H      -2.278336    -1.546263    -2.242198      24.76
 C      -2.899486    -2.931460    -0.684173     118.44
 O      -3.495699    -3.840498    -1.587349     235.30
 H      -2.731392    -4.269257    -2.188183      24.23
 H      -3.365718    -2.807060     0.306843      25.86
 H      -1.768338    -3.026131    -0.360595      23.62
 C       1.581480    -1.031701    -1.283241      23.98
 H       2.102915    -1.758851    -1.938051      22.47
 C       1.290491     1.113686    -0.075202      53.22
 H       1.724234     1.955933     0.235729      19.93
 C      -0.016763     0.773727    -0.036874      11.03
 O      -0.883601     1.651382     0.772998     174.04
 C      -0.279917     2.823263     1.283802      94.15
 H      -1.087320     3.403773     1.856111      22.18
 H       0.709504     2.709946     1.948506      23.66
 H       0.236527     3.520709     0.336678      20.57
 C      -0.655177    -0.483702    -0.423575       6.60
 O      -2.027308    -0.685791    -0.198757     144.27
 C       0.236800    -1.409137    -1.117963      67.18
 H      -0.020229    -2.327771    -1.507652      22.64
 C       2.214839     0.140082    -0.900271      18.88
 C       3.657943     0.500118    -1.078982      91.45
 H       3.851175     0.202764    -2.243536      22.11
 O       3.903242     1.911083    -0.876853     187.32
 H       4.734049     2.015350    -0.336592      18.14
 C       4.728885    -0.226901    -0.212698     101.71
 H       4.433585    -0.383995     0.829121      24.28
 O       4.786623    -1.699368    -0.436881     341.28
 H       5.127628    -1.836186    -1.335338      28.99
 C       6.166563     0.179577    -0.437668     105.93
 O       6.447056     1.589965    -0.245781     330.37
 H       6.861124     1.719176     0.622609      29.31
 H       6.250763    -0.045899    -1.518324      30.97
 H       6.777500    -0.440128     0.090751      31.33
55
name= lig-ACN-Water-frame_352
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 C      -4.017076     0.526629    -3.587560      43.47
 H      -4.370819    -0.302407    -4.125571      24.15
 C      -3.938412     1.859187    -1.433309      60.57
 H      -4.057857     1.783913    -0.341622      24.05
 C      -3.628117     2.971757    -2.176937      13.34
 O      -3.505968     4.236850    -1.584113     266.98
 C      -4.138418     4.502042    -0.235653      91.22
 H      -3.456774     4.180212     0.436057      33.04
 H      -5.185829     3.979841     0.045732      26.80
 H      -4.396948     5.445000    -0.216125      26.31
 C      -3.463410     3.003100    -3.552808      17.59
 O      -3.332680     4.087261    -4.287859     130.35
 H      -3.313692     4.921893    -3.557391      21.03
 C      -3.615131     1.778784    -4.275881      42.58
 H      -3.466086     1.859742    -5.377556      25.90
 C      -3.993242     0.597551    -2.130928       6.10
 C      -4.251339    -0.695872    -1.396116      50.36
 H      -4.832422    -1.295150    -1.936073      24.48
 O      -4.984778    -0.624320    -0.047665     152.78
 H      -4.349741    -0.176349     0.493108      29.64
 C      -2.824996    -1.375432    -1.198428      63.70
 H      -2.281666    -1.253082    -2.298700      25.76
 C      -2.892187    -2.872053    -0.681544     115.90
 O      -3.513135    -3.813656    -1.628714     204.06
 H      -2.858467    -4.187349    -2.257300      27.26
 H      -3.454390    -3.160224     0.221541      25.44
 H      -1.889781    -3.433850    -0.743735      22.79
 C       1.557036    -1.051784    -1.328058      57.58
 H       2.222928    -1.747746    -1.865385      19.81
 C       1.384569     0.957255    -0.114242      78.89
 H       1.673896     1.802219     0.191870      25.48
 C      -0.094073     0.761938    -0.022752      13.64
 O      -0.857679     1.608797     0.654300     196.84
 C      -0.254785     2.771224     1.308036     101.56
 H      -1.099053     3.262278     1.811106      24.64
 H       0.478889     2.333056     2.067939      24.50
 H       0.123517     3.673787     0.495805      21.40
 C      -0.656344    -0.440903    -0.509168      16.67
 O      -1.975249    -0.752820    -0.226364     199.27
 C       0.190924    -1.368014    -1.051163      60.90
 H      -0.295680    -2.251442    -1.515318      23.63
 C       2.134107     0.139788    -0.762480      32.43
 C       3.657717     0.472545    -1.025404      75.40
 H       3.989384     0.119688    -2.134869      21.78
 O       3.921354     1.920336    -0.929001     205.60
 H       4.780949     2.041373    -0.550263      17.99
 C       4.661510    -0.335927    -0.059190      91.48
 H       4.402722     0.031911     0.922038      24.04
 O       4.709957    -1.715371    -0.394638     341.63
 H       5.218480    -1.804161    -1.278580      25.82
 C       6.167629     0.166231    -0.425627     113.85
 O       6.497085     1.544760    -0.144668     391.27
 H       6.681607     1.735541     0.773816      33.12
 H       6.468172    -0.008188    -1.436257      30.26
 H       6.796677    -0.420705     0.158107      29.21
55
name= lig-ACN-Water-frame_353
 C      -4.005291     0.578671    -3.549984      68.33
 H      -3.892809    -0.380157    -4.045602      23.63
 C      -3.829616     1.758276    -1.470810      50.39
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 H      -4.004954     1.895601    -0.433090      20.94
 C      -3.598615     3.033843    -2.112508       1.21
 O      -3.477864     4.292567    -1.470055     223.12
 C      -4.098491     4.490956    -0.231011     116.10
 H      -3.583455     4.256171     0.667636      28.47
 H      -5.108747     3.892980    -0.304746      24.45
 H      -4.261591     5.442083    -0.168896      26.28
 C      -3.429514     2.977827    -3.606662       6.79
 O      -3.345719     4.234966    -4.332135     150.72
 H      -2.982833     5.106326    -3.823907      22.18
 C      -3.626400     1.705643    -4.252560      60.73
 H      -3.775246     1.640477    -5.336237      25.40
 C      -4.020358     0.531098    -2.146070      27.29
 C      -4.300596    -0.751932    -1.358015      98.76
 H      -4.898544    -1.339737    -1.908955      27.43
 O      -4.939097    -0.621050    -0.077509     167.05
 H      -4.306399    -0.507470     0.695282      25.75
 C      -2.843286    -1.466608    -1.216562      51.39
 H      -2.310652    -1.416754    -2.332732      25.98
 C      -2.842130    -2.910311    -0.766856     120.43
 O      -3.651750    -3.770825    -1.686468     193.56
 H      -3.095412    -4.060989    -2.391714      27.80
 H      -3.358684    -2.709985     0.185371      26.68
 H      -1.775167    -3.024042    -0.251691      23.66
 C       1.601332    -1.128465    -1.347188      31.71
 H       2.161978    -1.909082    -1.877027      20.94
 C       1.270241     0.994024    -0.073653      27.18
 H       1.743007     1.758221     0.339403      24.13
 C      -0.042250     0.723000     0.047137      23.09
 O      -0.936690     1.661241     0.579225     192.67
 C      -0.288892     2.725074     1.370400     103.07
 H      -1.065278     3.241400     1.874171      24.70
 H       0.521451     2.421509     2.088421      25.94
 H       0.381339     3.455488     0.566393      23.66
 C      -0.650401    -0.423387    -0.554964       5.55
 O      -1.981080    -0.717946    -0.202877     140.34
 C       0.225286    -1.353698    -1.151071      52.49
 H      -0.125411    -2.456968    -1.419174      22.62
 C       2.226558    -0.001969    -0.790485     -13.78
 C       3.672479     0.400362    -0.954243      87.19
 H       3.933355     0.049442    -2.101644      18.99
 O       3.891985     1.894473    -0.945739     215.50
 H       4.816809     2.008437    -0.693611      15.85
 C       4.699700    -0.303974    -0.072176     107.67
 H       4.490815    -0.382372     0.953054      24.05
 O       4.594019    -1.766490    -0.314137     304.93
 H       5.210117    -1.983475    -1.150050      25.89
 C       6.199312     0.112022    -0.299529     105.09
 O       6.488730     1.546510    -0.106677     395.20
 H       6.928282     1.680765     0.753760      28.85
 H       6.290664     0.017310    -1.329679      31.00
 H       6.837231    -0.609667     0.171330      27.89
55
name= lig-ACN-Water-frame_354
 C      -3.875971     0.530781    -3.488378      15.09
 H      -4.159145    -0.359870    -4.169868      19.08
 C      -3.760224     1.792053    -1.452707      58.46
 H      -3.696993     1.672736    -0.402514      20.14
 C      -3.526324     3.029395    -2.148034      14.98
 O      -3.387733     4.258501    -1.483361     236.41
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 C      -4.144587     4.496112    -0.164041      90.69
 H      -3.527246     3.995451     0.581999      26.04
 H      -5.144697     3.943860    -0.233666      24.48
 H      -4.338031     5.477196    -0.057287      24.90
 C      -3.474984     3.061143    -3.570231      27.75
 O      -3.337370     4.171205    -4.384526     200.91
 H      -3.193881     4.936646    -3.789203      23.25
 C      -3.672574     1.819010    -4.248395      33.02
 H      -3.508970     1.747577    -5.336673      23.92
 C      -4.120396     0.582481    -2.110950      36.55
 C      -4.182051    -0.842157    -1.339878     106.60
 H      -4.763407    -1.527373    -1.847208      28.27
 O      -4.884364    -0.615401    -0.069162     173.42
 H      -4.131947    -0.260297     0.545849      25.54
 C      -2.817223    -1.495852    -1.263609      79.49
 H      -2.244709    -1.387173    -2.339679      26.00
 C      -2.924571    -2.927510    -0.740397     117.17
 O      -3.722902    -3.682521    -1.674678     142.11
 H      -3.074806    -4.141441    -2.306571      27.08
 H      -3.537533    -3.124593     0.138039      26.36
 H      -1.987255    -3.680995    -0.883829      22.58
 C       1.660354    -1.189971    -1.331875      30.71
 H       2.285854    -1.895945    -1.873262      23.14
 C       1.415783     0.906163    -0.097935      51.91
 H       1.818829     1.819108     0.342077      20.53
 C      -0.095689     0.723688     0.048663     -26.46
 O      -1.011006     1.730933     0.595029     146.40
 C      -0.319043     2.706720     1.410147     102.13
 H      -1.074711     3.364959     1.782761      24.39
 H       0.235871     2.091419     2.136354      25.57
 H       0.333010     3.488783     0.655756      20.51
 C      -0.624293    -0.494512    -0.521727      -4.15
 O      -2.044238    -0.682021    -0.258761     140.87
 C       0.257747    -1.389699    -1.277575      88.17
 H      -0.216474    -2.455871    -1.668099      19.77
 C       2.180509     0.022155    -0.755220      46.00
 C       3.717996     0.381016    -0.976433      79.00
 H       4.035026    -0.052837    -2.091948      22.00
 O       3.812427     1.806603    -0.916971     192.61
 H       4.722954     2.081678    -0.509630      15.06
 C       4.745341    -0.367571     0.012046      87.17
 H       4.403841    -0.037273     0.948116      25.32
 O       4.517303    -1.818516    -0.265501     336.15
 H       5.027570    -2.091568    -1.075172      29.51
 C       6.215666     0.076680    -0.275914     111.91
 O       6.449126     1.495068    -0.109601     388.43
 H       6.767022     1.729335     0.806835      30.59
 H       6.473467    -0.229841    -1.232225      30.85
 H       6.929080    -0.389408     0.450162      27.12
55
name= lig-ACN-Water-frame_355
 C      -3.860105     0.635332    -3.552961      44.24
 H      -4.247849    -0.326802    -4.125693      19.96
 C      -3.750083     1.825261    -1.405807      40.80
 H      -3.530298     2.030553    -0.354074      18.45
 C      -3.504873     3.016899    -2.113367       4.09
 O      -3.319881     4.244181    -1.472610     227.94
 C      -4.141110     4.409445    -0.199747      92.12
 H      -3.594307     4.038664     0.759964      26.39
 H      -5.117498     4.002191    -0.258313      27.54
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 H      -4.123727     5.488003    -0.071243      25.26
 C      -3.570963     3.041784    -3.545374      12.06
 O      -3.314163     4.089781    -4.383542     109.62
 H      -3.505318     4.895931    -4.021843      23.36
 C      -3.656229     1.803859    -4.188945      57.11
 H      -3.485531     1.927102    -5.267326      23.45
 C      -4.034367     0.564493    -2.104874      15.37
 C      -4.153360    -0.745739    -1.408513      72.72
 H      -4.814468    -1.419952    -1.947085      26.96
 O      -4.765238    -0.631815    -0.029144     129.80
 H      -4.350801    -0.013730     0.562314      27.40
 C      -2.743684    -1.482681    -1.189653      73.32
 H      -2.277560    -1.584532    -2.301940      26.12
 C      -2.981995    -3.049801    -0.718528     110.62
 O      -3.837919    -3.635891    -1.749871     157.26
 H      -3.187051    -4.162343    -2.420658      25.51
 H      -3.232209    -2.995813     0.338706      27.59
 H      -1.777627    -3.307864    -0.543951      24.10
 C       1.642044    -1.170790    -1.328775      23.15
 H       2.300748    -1.831251    -1.875161      23.24
 C       1.297236     0.881951    -0.037387      46.28
 H       1.871206     1.876758     0.211777      20.01
 C      -0.058141     0.729947    -0.010216      13.39
 O      -0.983153     1.662404     0.557269     196.90
 C      -0.376526     2.712353     1.451605     102.05
 H      -1.205723     3.303890     1.888709      24.32
 H       0.122105     2.298606     2.356588      27.15
 H       0.508594     3.366239     0.918815      21.71
 C      -0.625348    -0.524295    -0.476121      10.13
 O      -1.994293    -0.657948    -0.372481     155.48
 C       0.240189    -1.416790    -1.266368      72.61
 H      -0.243612    -2.218021    -2.041101      20.98
 C       2.255858    -0.038522    -0.777436      15.16
 C       3.717452     0.301857    -0.981707      85.98
 H       4.080485     0.053998    -2.135356      22.99
 O       3.761255     1.769065    -0.879083     138.62
 H       4.684648     1.951421    -0.388335      16.14
 C       4.683363    -0.417237     0.003269      98.43
 H       4.529103    -0.284334     1.032383      25.76
 O       4.495993    -1.829074    -0.176705     339.86
 H       4.985136    -2.005853    -0.968165      30.62
 C       6.272780    -0.005421    -0.205250      90.98
 O       6.361110     1.462734    -0.169153     336.53
 H       6.777919     1.699500     0.761434      26.30
 H       6.717209    -0.274722    -1.137498      29.13
 H       6.812641    -0.588197     0.633119      27.86
55
name= lig-ACN-Water-frame_356
 C      -3.987034     0.604069    -3.487060      59.93
 H      -3.876793    -0.353903    -4.158678      22.86
 C      -3.729505     1.808105    -1.404709      60.79
 H      -3.847921     1.611492    -0.298398      22.14
 C      -3.558811     3.053249    -2.079931       5.47
 O      -3.300759     4.216369    -1.410386     289.68
 C      -4.045069     4.395974    -0.270743     107.59
 H      -3.681656     3.757263     0.647220      25.97
 H      -4.989028     4.044817    -0.522923      26.78
 H      -4.237640     5.519845    -0.062179      22.88
 C      -3.569707     2.994742    -3.507087      22.67
 O      -3.313048     4.096923    -4.369363     190.51
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 H      -3.403421     4.951033    -3.826565      23.97
 C      -3.620792     1.817770    -4.248889      41.87
 H      -3.771577     1.706781    -5.326463      26.51
 C      -3.827358     0.672514    -2.116672      37.44
 C      -4.110854    -0.678739    -1.326293      87.47
 H      -4.855298    -1.242836    -1.981895      23.90
 O      -4.684539    -0.641233    -0.043446     189.20
 H      -4.193216     0.044295     0.453416      26.73
 C      -2.809444    -1.571672    -1.238206      79.02
 H      -2.217750    -1.671333    -2.229191      26.37
 C      -2.941272    -2.943325    -0.693723     111.75
 O      -3.858812    -3.604120    -1.803248     102.91
 H      -3.230734    -4.026080    -2.455426      28.71
 H      -3.713849    -3.126162     0.032529      26.01
 H      -2.048898    -3.774938    -0.737270      23.94
 C       1.592938    -1.170368    -1.377140      40.11
 H       2.060833    -1.864969    -2.048473      22.21
 C       1.364853     0.860211    -0.092035      52.81
 H       1.659731     1.927805     0.455839      21.04
 C      -0.032594     0.655608     0.004961       0.19
 O      -0.892220     1.595256     0.559361     201.53
 C      -0.439935     2.654228     1.495859     105.74
 H      -1.396330     3.297385     1.518568      22.51
 H       0.015927     2.190989     2.411716      25.82
 H       0.206559     3.395736     0.885237      23.12
 C      -0.590925    -0.512239    -0.545805      18.13
 O      -1.917471    -0.611030    -0.395180     138.04
 C       0.244923    -1.390003    -1.224469      56.83
 H      -0.213790    -2.289876    -1.779982      22.64
 C       2.156973    -0.061957    -0.722438      28.35
 C       3.658231     0.306126    -0.941590     101.55
 H       3.895241    -0.173327    -2.057325      23.60
 O       3.783553     1.750086    -0.832986     184.19
 H       4.673716     1.955046    -0.410968      17.28
 C       4.725332    -0.438363    -0.027071     103.79
 H       4.283020    -0.122438     0.894270      27.17
 O       4.531760    -1.875342    -0.116959     294.24
 H       4.944024    -2.313310    -0.949185      28.53
 C       6.193602    -0.086572    -0.124401      90.74
 O       6.321261     1.410313    -0.192525     318.86
 H       6.837203     1.802734     0.631478      26.60
 H       6.571921    -0.557946    -1.059696      28.29
 H       6.875396    -0.411767     0.786106      27.20
55
name= lig-ACN-Water-frame_357
 C      -3.908548     0.590907    -3.518750      45.73
 H      -4.215223    -0.442069    -3.892815      22.02
 C      -3.714751     1.852849    -1.371236      39.62
 H      -3.790731     2.033664    -0.223293      17.97
 C      -3.568619     3.015993    -2.111843      26.53
 O      -3.213203     4.232792    -1.460193     262.11
 C      -4.118687     4.407540    -0.236971      89.24
 H      -3.586088     3.821714     0.643534      23.20
 H      -5.069547     4.132355    -0.331260      26.86
 H      -3.891829     5.544538     0.123328      21.99
 C      -3.468731     3.014960    -3.557197      13.63
 O      -3.333024     4.153011    -4.280285     108.00
 H      -3.476444     5.045895    -3.627949      24.09
 C      -3.747331     1.740527    -4.231144      51.82
 H      -3.623654     1.880359    -5.298327      22.16
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 C      -3.792077     0.560417    -2.079197      22.45
 C      -4.010859    -0.719180    -1.356677      76.07
 H      -4.870502    -1.329709    -1.913961      22.92
 O      -4.645784    -0.574480    -0.024440     142.45
 H      -4.040469    -0.306806     0.789782      22.96
 C      -2.733725    -1.488632    -1.295048      84.11
 H      -2.409395    -1.539011    -2.359170      27.65
 C      -3.106060    -2.977674    -0.776790     116.42
 O      -3.808119    -3.563698    -1.843097     230.74
 H      -3.157460    -3.879655    -2.437253      29.38
 H      -3.456598    -2.851637     0.269291      25.67
 H      -1.994040    -3.444279    -0.475637      24.00
 C       1.618171    -1.168977    -1.431569      39.88
 H       2.344951    -1.765981    -1.975494      18.41
 C       1.393980     0.877706    -0.070201      51.42
 H       2.140429     1.745103     0.450465      19.80
 C       0.039502     0.647755     0.082562      22.87
 O      -0.870188     1.518257     0.598927     204.67
 C      -0.518822     2.599775     1.424697     124.62
 H      -1.494506     3.170998     1.772038      23.43
 H      -0.232899     2.207813     2.474787      26.30
 H       0.299729     3.263981     1.104266      25.14
 C      -0.583003    -0.477013    -0.608542       1.49
 O      -1.990167    -0.647558    -0.386635     146.77
 C       0.179923    -1.477889    -1.259727      59.82
 H      -0.211301    -2.457070    -1.466668      22.84
 C       2.202861    -0.054303    -0.746519      20.80
 C       3.637419     0.284562    -0.965205      86.75
 H       3.914606     0.171371    -2.156101      19.62
 O       3.831784     1.729358    -0.803892     213.14
 H       4.719262     1.804943    -0.498514      18.51
 C       4.614685    -0.470441     0.047711      93.68
 H       4.438580    -0.283991     1.103233      23.23
 O       4.567649    -1.943393    -0.073404     290.76
 H       5.124030    -1.991242    -0.954970      24.59
 C       6.130512    -0.060233    -0.085799      84.31
 O       6.344390     1.344987    -0.205363     387.91
 H       6.573764     1.623260     0.714723      30.70
 H       6.747175    -0.533698    -0.965737      25.86
 H       6.592412    -0.538237     0.923457      25.31
55
name= lig-ACN-Water-frame_358
 C      -3.815707     0.535403    -3.457012      31.17
 H      -4.249482    -0.186734    -4.117242      21.60
 C      -3.697316     1.808429    -1.430740      72.14
 H      -3.557880     1.785040    -0.292008      21.55
 C      -3.446415     2.997973    -2.150587      11.66
 O      -3.256054     4.248297    -1.495085     221.19
 C      -4.038930     4.461631    -0.201456     101.05
 H      -3.773723     3.740812     0.660877      24.48
 H      -5.004573     4.398541    -0.467880      26.46
 H      -3.941262     5.710673     0.002585      22.32
 C      -3.468784     2.966674    -3.559740      33.88
 O      -3.342860     4.227758    -4.210746     145.33
 H      -3.546765     5.028994    -3.516638      19.20
 C      -3.782638     1.803393    -4.213450      42.85
 H      -3.858830     1.640617    -5.269720      22.89
 C      -3.906754     0.615901    -2.043708      38.27
 C      -4.067569    -0.720144    -1.341299      88.84
 H      -4.735030    -1.506326    -2.003393      25.36
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 O      -4.625860    -0.517118     0.005995     168.04
 H      -3.810573    -0.463126     0.560552      27.08
 C      -2.701707    -1.473429    -1.298602      95.93
 H      -2.077573    -1.514308    -2.149083      29.28
 C      -3.051594    -2.854033    -0.808286     106.49
 O      -3.804993    -3.587794    -1.861164     164.58
 H      -3.094362    -4.001085    -2.423724      28.68
 H      -3.918553    -2.882294    -0.105304      25.28
 H      -2.092417    -3.574493    -0.580344      24.76
 C       1.616520    -1.188041    -1.424312      42.02
 H       2.170663    -1.985536    -1.932303      22.85
 C       1.464070     0.839092     0.020659      24.71
 H       1.868993     1.902800     0.505800      20.17
 C       0.069326     0.629270     0.052860     -22.40
 O      -0.966406     1.447283     0.651004     155.95
 C      -0.547151     2.570882     1.499197     109.80
 H      -1.515980     3.248804     1.424442      22.74
 H      -0.082446     2.191542     2.514124      25.70
 H       0.123426     3.144074     0.944608      25.81
 C      -0.610774    -0.541317    -0.592553     -12.44
 O      -1.944093    -0.698278    -0.358452     163.18
 C       0.248267    -1.506025    -1.275423      64.26
 H      -0.146742    -2.353409    -1.707768      25.00
 C       2.206458    -0.044503    -0.897074      14.08
 C       3.708467     0.273800    -0.975591      82.14
 H       4.214385    -0.300007    -1.959048      21.48
 O       3.881808     1.724937    -0.775077     186.14
 H       4.821220     1.877931    -0.642823      17.51
 C       4.541670    -0.504773     0.095533      78.71
 H       3.931862    -0.324209     1.015701      24.77
 O       4.596953    -1.943065    -0.099051     284.89
 H       5.185302    -2.234649    -0.787914      29.43
 C       6.075021    -0.104486    -0.036612      85.82
 O       6.408547     1.337213    -0.155994     311.46
 H       6.558601     1.771508     0.667129      31.57
 H       6.462551    -0.655266    -1.046517      25.83
 H       6.716391    -0.493135     0.910362      26.24
55
name= lig-ACN-Water-frame_359
 C      -3.893385     0.603866    -3.500988      71.90
 H      -3.812730    -0.337832    -3.878113      24.22
 C      -3.632968     1.796873    -1.407160      52.33
 H      -3.668240     1.774509    -0.312946      22.64
 C      -3.352608     3.001754    -2.070213       8.00
 O      -3.314781     4.244591    -1.493125     266.01
 C      -3.972660     4.533244    -0.317968     109.82
 H      -3.650405     3.865353     0.528253      25.75
 H      -5.028083     4.427465    -0.353193      26.68
 H      -3.552442     5.663786     0.132829      23.42
 C      -3.511508     3.076854    -3.520351      -0.60
 O      -3.368487     4.228020    -4.192487     115.36
 H      -3.178421     4.991513    -3.594126      22.24
 C      -3.697582     1.782162    -4.215687      49.73
 H      -3.957504     1.869881    -5.243104      22.70
 C      -4.009137     0.596883    -2.142784      43.94
 C      -4.126000    -0.665486    -1.340351      78.84
 H      -5.063594    -1.328740    -1.830243      23.50
 O      -4.597880    -0.514844    -0.010719     167.01
 H      -4.039126    -0.162588     0.668350      26.52
 C      -2.716601    -1.448510    -1.288563      83.16
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 H      -2.419322    -1.444131    -2.253847      30.16
 C      -3.033823    -2.891158    -0.810642     105.94
 O      -3.808218    -3.631740    -1.897172     172.57
 H      -3.070776    -4.041587    -2.557085      25.38
 H      -3.596007    -2.731646     0.161616      25.87
 H      -2.095627    -3.463276    -0.357657      24.90
 C       1.674605    -1.219268    -1.439290      48.19
 H       2.266395    -1.865477    -2.125741      22.49
 C       1.394130     0.750346    -0.030935      52.44
 H       1.883396     1.679130     0.497342      22.33
 C      -0.025185     0.552190     0.025590       8.74
 O      -1.012924     1.363248     0.734527     152.60
 C      -0.551438     2.568845     1.466569     113.34
 H      -1.465718     3.240297     1.756693      23.89
 H      -0.242982     2.282322     2.609980      25.50
 H       0.177624     3.082649     1.002917      26.88
 C      -0.478752    -0.614890    -0.519679      33.45
 O      -1.858212    -0.743614    -0.279778     160.69
 C       0.239007    -1.461304    -1.262401      78.61
 H      -0.124703    -2.281492    -1.813830      24.33
 C       2.237049     0.027935    -0.909317      19.00
 C       3.772862     0.230213    -0.983032      74.20
 H       4.126428     0.116139    -2.162605      22.78
 O       3.931958     1.681787    -0.815732     172.87
 H       4.886722     1.869895    -0.530317      17.73
 C       4.564705    -0.516048     0.117253      91.42
 H       4.190732    -0.342607     1.189570      24.06
 O       4.552843    -1.953482    -0.125037     286.26
 H       5.200617    -2.014822    -0.840399      28.63
 C       6.032953    -0.074259     0.082445      76.27
 O       6.452787     1.333867    -0.114764     306.78
 H       6.928240     1.556271     0.758997      27.81
 H       6.367463    -0.484542    -1.032620      25.12
 H       6.744757    -0.679707     0.809476      26.21
55
name= lig-ACN-Water-frame_360
 C      -3.969706     0.637711    -3.605681      39.15
 H      -4.055870    -0.174214    -4.213984      23.89
 C      -3.639679     1.804779    -1.369341      74.00
 H      -3.763615     1.857443    -0.337710      21.46
 C      -3.419777     2.985336    -2.060122       8.97
 O      -3.261434     4.295848    -1.562810     236.10
 C      -3.933448     4.566289    -0.263777      94.34
 H      -3.551447     3.905438     0.499786      27.71
 H      -5.002637     4.684869    -0.372285      26.12
 H      -3.607046     5.792039    -0.106599      23.58
 C      -3.493471     3.023068    -3.454371      23.19
 O      -3.397971     4.231365    -4.226701     191.12
 H      -3.169928     4.991649    -3.782573      23.21
 C      -3.632643     1.914296    -4.233405      39.50
 H      -3.333916     2.002353    -5.274495      23.79
 C      -3.971859     0.657209    -2.087502       1.63
 C      -4.097687    -0.637278    -1.305311      79.65
 H      -4.795777    -1.492705    -1.908594      21.51
 O      -4.655758    -0.487735     0.034526     150.37
 H      -4.025393     0.161216     0.505051      26.12
 C      -2.798936    -1.434013    -1.288069      75.14
 H      -2.241392    -1.390220    -2.106336      29.17
 C      -3.044561    -2.973918    -0.813964     106.84
 O      -3.786848    -3.645875    -1.832391     198.48
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 H      -2.996396    -3.907128    -2.486862      26.26
 H      -3.678066    -3.064835     0.113914      24.73
 H      -2.001926    -3.430002    -0.842902      24.69
 C       1.722163    -1.152370    -1.514111      21.66
 H       2.389850    -1.727662    -2.192106      23.39
 C       1.318240     0.800222    -0.105578      59.82
 H       1.843205     1.573193     0.454831      24.35
 C      -0.008403     0.568669     0.142946       9.29
 O      -0.970156     1.303422     0.811601     204.92
 C      -0.548609     2.528570     1.468738     110.57
 H      -1.529192     3.111512     1.531182      22.97
 H       0.025931     2.136273     2.483884      24.03
 H       0.086422     3.027340     0.920413      27.77
 C      -0.563915    -0.664024    -0.454020     -24.47
 O      -1.892547    -0.864062    -0.267636     137.82
 C       0.385164    -1.514789    -1.353016      58.41
 H      -0.153574    -2.434402    -1.688554      21.36
 C       2.239640    -0.093928    -0.849575      22.14
 C       3.699743     0.309899    -0.963452      87.82
 H       4.146779    -0.364839    -1.926797      23.69
 O       3.987921     1.688313    -0.876439     169.14
 H       4.817055     1.803831    -0.226586      14.64
 C       4.606916    -0.491262     0.124624      83.16
 H       4.080818    -0.354833     1.159163      25.32
 O       4.516054    -1.925481    -0.151205     261.16
 H       4.961315    -2.174606    -1.065636      26.71
 C       6.137828    -0.082879     0.031519      85.56
 O       6.476344     1.321289     0.013210     299.73
 H       7.025644     1.645693     0.882350      25.62
 H       6.651786    -0.673855    -0.900738      25.95
 H       6.559122    -0.492416     1.014195      26.64
55
name= lig-ACN-Water-frame_361
 C      -3.976761     0.745442    -3.547429      64.23
 H      -4.508132     0.000682    -4.070313      25.65
 C      -3.712143     1.849203    -1.360921      41.70
 H      -3.596984     1.782239    -0.325118      21.02
 C      -3.537633     3.113745    -2.085765      29.95
 O      -3.216153     4.333969    -1.546869     251.78
 C      -3.852564     4.662287    -0.255748      94.95
 H      -3.623711     4.054042     0.577246      27.75
 H      -4.948958     4.393681    -0.428657      23.12
 H      -3.589956     5.798738     0.079652      22.42
 C      -3.424933     3.102108    -3.517864      20.75
 O      -3.412450     4.204503    -4.254444     199.86
 H      -3.414540     5.012674    -3.678162      27.97
 C      -3.567497     1.888461    -4.248690      53.30
 H      -3.384681     1.821344    -5.356172      24.84
 C      -3.916992     0.660220    -2.169030      20.24
 C      -4.095744    -0.653025    -1.308195      45.94
 H      -4.994070    -1.283615    -1.915413      23.19
 O      -4.708859    -0.420863     0.023378     152.75
 H      -4.042446    -0.183879     0.827875      20.21
 C      -2.774862    -1.548551    -1.200532      99.58
 H      -2.489146    -1.568870    -2.158248      28.70
 C      -2.995927    -2.974263    -0.857336     118.80
 O      -3.821752    -3.699361    -1.804969     249.48
 H      -3.286177    -3.969747    -2.549761      30.71
 H      -3.442780    -3.068437     0.167960      25.92
 H      -2.007004    -3.438433    -0.642387      25.69
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 C       1.703646    -1.163521    -1.605345      36.31
 H       2.322538    -1.858390    -2.220212      19.28
 C       1.394304     0.870764    -0.079097      60.30
 H       1.690483     1.791616     0.220210      23.03
 C      -0.021067     0.395687     0.157668       7.25
 O      -0.908494     1.240552     0.874370     166.41
 C      -0.507033     2.493375     1.459986     117.25
 H      -1.388018     3.074437     1.725986      24.74
 H       0.060781     2.520977     2.569889      23.75
 H      -0.031840     3.066513     0.785387      27.15
 C      -0.529189    -0.721747    -0.533357      18.87
 O      -1.938446    -0.973967    -0.215884     192.77
 C       0.324571    -1.521465    -1.301944      60.74
 H       0.123902    -2.489329    -1.885212      21.78
 C       2.192494     0.000096    -0.763273      11.43
 C       3.707457     0.243293    -0.877700      79.15
 H       3.958407     0.077702    -2.109429      20.84
 O       4.003412     1.743896    -0.937654     182.87
 H       4.893135     1.876279    -0.430617      17.29
 C       4.651454    -0.463124     0.029740      94.59
 H       4.383955    -0.241777     1.153419      22.26
 O       4.483422    -1.882227    -0.167770     277.86
 H       4.773142    -1.972739    -1.179846      25.15
 C       6.234721    -0.140108     0.080173      77.48
 O       6.468033     1.339784     0.102045     343.21
 H       6.882029     1.522193     1.086592      24.26
 H       6.772084    -0.616480    -0.874627      26.65
 H       6.702345    -0.624810     0.949226      27.65
55
name= lig-ACN-Water-frame_362
 C      -3.983159     0.729426    -3.500462      36.58
 H      -4.200338    -0.243210    -4.041618      23.91
 C      -3.729093     1.967344    -1.470956      68.41
 H      -3.629611     1.975469    -0.379188      23.10
 C      -3.578412     3.139061    -2.126382      13.98
 O      -3.174934     4.400927    -1.462588     269.55
 C      -3.830009     4.691612    -0.262199     100.25
 H      -3.276387     4.179028     0.498700      27.53
 H      -4.991143     4.629797    -0.201309      24.30
 H      -3.731940     5.837022    -0.132369      23.60
 C      -3.435036     3.105363    -3.556674       1.51
 O      -3.388349     4.296155    -4.323046     151.14
 H      -3.323518     5.197046    -3.695870      21.02
 C      -3.531234     1.850525    -4.241075      44.82
 H      -3.897870     1.983029    -5.312453      23.52
 C      -3.894180     0.687551    -2.036459      22.03
 C      -4.129079    -0.634028    -1.300796      80.97
 H      -4.945691    -1.371096    -1.898708      22.67
 O      -4.750732    -0.364061    -0.036311     181.67
 H      -4.011251    -0.306403     0.622826      24.84
 C      -2.822465    -1.580563    -1.269196      64.99
 H      -2.232832    -1.461517    -2.085675      28.02
 C      -2.980240    -3.090687    -0.771731     110.58
 O      -3.893199    -3.770399    -1.778203     209.59
 H      -3.234017    -3.980146    -2.421792      31.32
 H      -3.550235    -3.054932     0.177175      25.63
 H      -2.028678    -3.572729    -0.776254      26.81
 C       1.616053    -1.062791    -1.424916      30.23
 H       2.295282    -1.624763    -2.073731      24.85
 C       1.308760     0.812712    -0.000497      66.75
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 H       1.656378     1.667832     0.331358      26.11
 C       0.060067     0.420311     0.139857      27.05
 O      -0.853813     1.121042     0.939637     168.37
 C      -0.462115     2.526880     1.435712     106.74
 H      -1.404476     2.855411     1.756110      26.57
 H       0.397274     2.212017     2.265034      23.85
 H      -0.013046     3.150852     0.701126      26.74
 C      -0.565288    -0.767598    -0.512051     -16.88
 O      -1.847003    -1.039827    -0.168851     137.78
 C       0.302259    -1.559113    -1.361338      52.33
 H      -0.289754    -2.381162    -1.865714      18.64
 C       2.251009     0.001690    -0.866712      15.62
 C       3.766876     0.378825    -1.002253      81.44
 H       4.088172    -0.275626    -2.086182      22.68
 O       3.978075     1.780810    -0.944413     189.37
 H       4.885807     1.877568    -0.644917      21.93
 C       4.763438    -0.469043     0.069559      82.93
 H       4.273139    -0.274895     1.121608      24.72
 O       4.466128    -1.857756    -0.207182     322.71
 H       4.847418    -2.085196    -1.101103      28.33
 C       6.257512    -0.120382     0.049995      97.14
 O       6.422810     1.295176     0.152138     347.31
 H       7.051415     1.644262     0.921697      25.54
 H       6.731360    -0.356506    -0.971553      28.94
 H       6.719433    -0.678948     0.806245      29.00
55
name= lig-ACN-Water-frame_363
 C      -3.857658     0.653469    -3.439631      44.23
 H      -3.892667    -0.342570    -4.080400      20.86
 C      -3.718005     1.995174    -1.401381      36.38
 H      -3.888735     2.204753    -0.284769      17.56
 C      -3.456286     3.251784    -2.196859      18.87
 O      -3.190020     4.376530    -1.531866     152.80
 C      -3.805391     4.788310    -0.167575      86.43
 H      -3.424150     4.388284     0.763772      26.30
 H      -4.928277     4.341791    -0.235011      21.58
 H      -3.695800     5.842136    -0.185372      25.59
 C      -3.497946     3.205196    -3.609188       7.89
 O      -3.338523     4.322951    -4.374553     -15.62
 H      -3.439826     5.227674    -3.718216      20.50
 C      -3.692232     1.899270    -4.181979      28.24
 H      -3.545570     1.773390    -5.345296      21.92
 C      -3.921034     0.738718    -2.070637      24.06
 C      -4.086287    -0.620831    -1.314020      62.33
 H      -4.838478    -1.217944    -2.087032      23.99
 O      -4.781220    -0.363827    -0.076832     189.55
 H      -4.254876     0.079142     0.565159      28.09
 C      -2.781385    -1.574649    -1.209703      73.43
 H      -2.441871    -1.631503    -2.234748      29.36
 C      -3.092025    -3.125333    -0.792409     116.45
 O      -3.918086    -3.839888    -1.706255     184.41
 H      -3.372172    -4.172227    -2.529162      27.64
 H      -3.523986    -3.241607     0.217642      27.10
 H      -2.157143    -3.582278    -0.720442      27.63
 C       1.649619    -1.136329    -1.426808      42.99
 H       2.211037    -1.753575    -2.121217      21.24
 C       1.468670     0.768236    -0.006245      54.34
 H       1.766913     1.467902     0.682953      26.39
 C      -0.025698     0.399649     0.136545      -4.26
 O      -0.803616     1.099805     1.010056     200.21
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 C      -0.411694     2.390401     1.386280     118.39
 H      -1.147659     2.873422     1.942915      27.14
 H       0.512279     2.538363     2.197859      23.59
 H      -0.316766     2.998666     0.455385      25.61
 C      -0.521469    -0.755811    -0.446584      31.56
 O      -1.852436    -1.097308    -0.149892     161.22
 C       0.244095    -1.460543    -1.334424      69.88
 H       0.155962    -2.359917    -1.913948      22.15
 C       2.255826     0.098561    -0.845102      35.47
 C       3.808665     0.369834    -1.059505      67.53
 H       4.351380     0.167941    -2.237912      21.95
 O       3.957485     1.829638    -0.958483     212.83
 H       4.736713     2.060669    -0.427151      19.84
 C       4.679120    -0.450967     0.044687      81.12
 H       4.340027    -0.229493     1.139981      23.47
 O       4.503553    -1.861285    -0.225975     319.46
 H       4.907315    -2.054344    -1.083532      29.16
 C       6.250154    -0.119712    -0.048180     100.92
 O       6.386108     1.325486     0.155293     346.44
 H       6.768907     1.450135     1.098254      26.45
 H       6.621711    -0.559490    -0.997989      30.30
 H       6.854363    -0.545906     0.668285      29.55
55
name= lig-ACN-Water-frame_364
 C      -3.702717     0.774991    -3.457213      33.08
 H      -3.840395    -0.306536    -3.975560      20.15
 C      -3.729148     2.047806    -1.435124      68.45
 H      -3.841075     2.014674    -0.281975      19.98
 C      -3.418882     3.150384    -2.112107      -0.63
 O      -3.188364     4.478281    -1.526497     264.83
 C      -3.791145     4.818882    -0.219583      97.41
 H      -3.082963     4.411039     0.551427      26.42
 H      -4.963957     4.419803    -0.153116      24.66
 H      -3.891045     5.797542    -0.155144      26.96
 C      -3.565323     3.207707    -3.593593       5.58
 O      -3.301025     4.311558    -4.430425     145.72
 H      -3.398913     5.273700    -3.943008      17.78
 C      -3.791174     1.929871    -4.198370      53.93
 H      -3.460141     1.834429    -5.311005      22.73
 C      -3.858864     0.766732    -2.047347      41.59
 C      -4.014129    -0.565369    -1.312663      89.40
 H      -4.784513    -1.307794    -1.852052      23.87
 O      -4.829255    -0.399286    -0.087464     177.35
 H      -4.251225     0.041513     0.604606      25.59
 C      -2.832733    -1.604141    -1.140297      85.23
 H      -2.175701    -1.606425    -2.057775      25.53
 C      -3.133188    -3.070124    -0.776348     113.81
 O      -3.978442    -3.926886    -1.674398     164.30
 H      -3.306872    -4.079850    -2.456282      28.46
 H      -3.738511    -2.993383     0.150281      26.19
 H      -2.212586    -3.545480    -0.661237      27.03
 C       1.751010    -1.121325    -1.552757      -6.04
 H       2.314707    -1.829207    -2.140911      20.59
 C       1.422878     0.754398     0.068331      47.67
 H       1.979431     1.584044     0.564669      19.71
 C       0.126567     0.407918     0.191097       4.84
 O      -0.782012     1.045365     1.113221     201.17
 C      -0.375612     2.421106     1.363515     106.30
 H      -1.145376     2.739015     1.971468      25.58
 H       0.767426     2.345262     1.799382      22.13
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 H      -0.263629     3.075197     0.374023      23.70
 C      -0.556805    -0.732852    -0.459634     -19.61
 O      -1.897349    -1.129792    -0.138296     146.34
 C       0.384838    -1.426433    -1.305480      54.98
 H      -0.138207    -2.220245    -1.671736      19.96
 C       2.316453    -0.046839    -0.919454      -2.36
 C       3.782159     0.397381    -0.984401      71.45
 H       3.963474    -0.074690    -2.195649      20.44
 O       3.926901     1.872862    -0.952101     225.82
 H       4.709020     2.083187    -0.296150      15.96
 C       4.666694    -0.434033    -0.076850      94.50
 H       4.238807    -0.198897     0.962021      23.22
 O       4.536719    -1.865509    -0.211178     333.10
 H       4.704543    -1.983933    -1.181455      28.06
 C       6.153882    -0.097363    -0.099526      97.95
 O       6.370367     1.373463     0.119162     359.24
 H       6.858776     1.600769     0.972594      29.35
 H       6.547862    -0.111971    -1.065727      30.23
 H       6.561586    -0.766051     0.571747      29.85
55
name= lig-ACN-Water-frame_365
 C      -3.692928     0.815089    -3.469554      44.53
 H      -3.648503    -0.179140    -4.115932      25.01
 C      -3.733515     1.984854    -1.353440      34.41
 H      -3.651365     2.091205    -0.228645      22.76
 C      -3.486360     3.307786    -2.132703      -3.77
 O      -3.203356     4.534993    -1.558451     248.56
 C      -3.749030     4.806566    -0.304088     109.84
 H      -3.137508     4.424331     0.591700      27.43
 H      -4.834765     4.260511    -0.036982      25.52
 H      -3.794479     5.768140    -0.273406      28.39
 C      -3.549025     3.213982    -3.535951      11.09
 O      -3.308635     4.240636    -4.409606     171.28
 H      -3.093712     5.050262    -3.916515      22.24
 C      -3.690157     2.025282    -4.259137      60.80
 H      -4.033216     2.105936    -5.311848      21.77
 C      -3.700515     0.762689    -2.031853      17.95
 C      -4.066538    -0.606213    -1.286282      77.68
 H      -4.715526    -1.029981    -2.136091      24.50
 O      -4.820015    -0.413707    -0.073287     160.65
 H      -4.126643    -0.364390     0.734079      22.09
 C      -2.814821    -1.540980    -1.204088      63.27
 H      -2.370031    -1.543274    -2.321771      25.09
 C      -3.222410    -3.044501    -0.677953      94.53
 O      -3.973211    -3.938136    -1.672392     203.60
 H      -3.427076    -4.090792    -2.411504      32.59
 H      -3.854489    -3.049204     0.268077      24.22
 H      -2.272574    -3.529546    -0.440284      25.33
 C       1.759004    -1.118189    -1.632750      40.09
 H       2.401091    -1.628852    -2.356301      19.60
 C       1.501298     0.635731    -0.016272      57.80
 H       1.842714     1.690519     0.364109      21.02
 C       0.070245     0.330620     0.321029      26.82
 O      -0.697056     1.021649     1.161313     194.40
 C      -0.330694     2.480397     1.383202      92.78
 H      -0.926788     2.978988     2.179680      25.23
 H       0.731807     2.582141     1.880445      22.68
 H      -0.493087     3.057405     0.335506      24.25
 C      -0.442501    -0.678729    -0.482804       2.55
 O      -1.812175    -1.090811    -0.085394     139.61
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 C       0.374462    -1.521618    -1.316642      54.85
 H       0.101513    -2.329791    -1.834828      23.09
 C       2.275613    -0.041229    -0.820428      41.19
 C       3.682396     0.392844    -1.069512      76.35
 H       4.249123     0.207572    -2.211161      20.96
 O       3.872232     1.821459    -0.914879     208.43
 H       4.837482     1.984855    -0.595037      20.64
 C       4.642157    -0.386539    -0.054721      89.27
 H       4.348416    -0.223887     1.013298      25.65
 O       4.532230    -1.841287    -0.217458     298.65
 H       4.783320    -2.184377    -1.131068      27.78
 C       6.108894     0.027985    -0.201283     116.44
 O       6.379186     1.413729     0.130613     301.10
 H       6.944521     1.403677     0.932225      26.58
 H       6.447203    -0.355675    -1.085029      33.11
 H       6.752106    -0.470996     0.499343      29.20
55
name= lig-ACN-Water-frame_366
 C      -3.697834     0.795756    -3.506692      57.78
 H      -3.865499    -0.164011    -4.068598      23.07
 C      -3.611507     2.113701    -1.346107      59.78
 H      -3.761664     2.065066    -0.282365      23.85
 C      -3.590829     3.246177    -2.091880      27.27
 O      -3.218856     4.532521    -1.650578     248.01
 C      -3.721835     4.827383    -0.250498     108.28
 H      -3.008762     4.403599     0.549476      24.07
 H      -4.819480     4.328346    -0.341958      22.21
 H      -3.830036     5.802471    -0.078123      26.93
 C      -3.475197     3.241511    -3.511853      14.90
 O      -3.306125     4.291050    -4.360779     182.20
 H      -3.295830     5.095797    -3.908235      25.48
 C      -3.618307     1.972850    -4.156150      48.02
 H      -3.559849     1.988398    -5.234025      27.29
 C      -3.635205     0.809481    -2.051337     -16.40
 C      -4.035078    -0.564573    -1.356815      68.19
 H      -4.792033    -1.209179    -1.839978      24.14
 O      -4.768133    -0.446148    -0.060947     158.56
 H      -4.120760    -0.191528     0.715885      24.06
 C      -2.814449    -1.563904    -1.140079      51.72
 H      -2.223357    -1.768430    -2.206979      25.25
 C      -3.269796    -3.038374    -0.676672     106.27
 O      -3.922474    -3.849437    -1.644954     190.26
 H      -3.212039    -4.021723    -2.298226      30.25
 H      -4.019751    -2.822403     0.147279      24.30
 H      -2.316842    -3.496795    -0.254159      26.38
 C       1.678470    -1.129081    -1.601711      26.75
 H       2.172591    -1.619266    -2.465597      24.32
 C       1.420554     0.672849     0.064115      41.02
 H       1.945328     1.577773     0.614230      21.21
 C       0.178408     0.272180     0.299082       7.57
 O      -0.628948     1.103645     1.263520     186.60
 C      -0.304195     2.476654     1.438390     105.86
 H      -1.208445     2.742491     2.099515      24.22
 H       0.750554     2.604922     1.736582      25.19
 H      -0.433386     3.114772     0.329619      24.63
 C      -0.435225    -0.846893    -0.461694     -18.29
 O      -1.742238    -1.038707    -0.156379     122.05
 C       0.376032    -1.573792    -1.400027      50.00
 H      -0.064482    -2.380443    -1.901203      24.18
 C       2.260383    -0.070947    -0.938664      12.65
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 C       3.737180     0.354985    -1.114195      84.38
 H       3.884142    -0.068767    -2.313162      22.81
 O       3.813085     1.785182    -0.877405     217.24
 H       4.727980     2.020900    -0.724338      22.71
 C       4.602341    -0.364865    -0.029993      90.26
 H       4.217278    -0.043362     0.931287      27.09
 O       4.524400    -1.789499    -0.176159     289.02
 H       4.696434    -1.822909    -1.184557      27.03
 C       6.174774     0.055087    -0.241100      95.69
 O       6.414359     1.484171     0.112028     284.90
 H       6.782789     1.595382     1.037652      27.37
 H       6.431193     0.093698    -1.212427      32.30
 H       6.697932    -0.711976     0.376457      28.95
55
name= lig-ACN-Water-frame_367
 C      -3.692469     0.721939    -3.409993      21.93
 H      -3.981190    -0.174368    -3.878066      16.74
 C      -3.535961     2.022973    -1.376408      56.15
 H      -3.584041     2.124145    -0.352233      20.77
 C      -3.513435     3.298124    -2.129190       2.02
 O      -3.290263     4.560941    -1.605689     249.23
 C      -3.713999     4.815365    -0.288777     112.70
 H      -3.004350     4.256866     0.431324      24.29
 H      -4.769703     4.486879     0.137352      24.11
 H      -3.596920     5.885687    -0.277875      25.94
 C      -3.455519     3.181704    -3.551233      15.38
 O      -3.304842     4.390909    -4.292638     158.90
 H      -3.278065     5.174829    -3.766051      20.63
 C      -3.499817     1.956132    -4.185409      57.95
 H      -3.136118     1.895656    -5.163842      29.34
 C      -3.737260     0.809750    -2.003287      37.36
 C      -3.914815    -0.527072    -1.297292      92.08
 H      -4.483974    -0.945100    -2.093582      27.06
 O      -4.691370    -0.444214    -0.078911     203.05
 H      -4.212634     0.096844     0.557238      26.59
 C      -2.748708    -1.615290    -1.116552      76.48
 H      -2.185081    -1.760230    -2.244596      25.19
 C      -3.275047    -2.926238    -0.579317     107.25
 O      -3.834808    -3.740978    -1.670783     148.42
 H      -3.103283    -4.067584    -2.380314      25.77
 H      -4.103423    -2.894287     0.199793      25.39
 H      -2.410554    -3.556182    -0.089907      25.83
 C       1.655009    -1.155701    -1.665001      35.72
 H       2.355853    -1.724601    -2.328964      20.79
 C       1.539004     0.639737     0.052016      46.42
 H       2.031749     1.397371     0.731087      23.09
 C       0.148864     0.283856     0.304642     -28.01
 O      -0.579268     0.990728     1.273691     170.46
 C      -0.315466     2.457853     1.448732      94.14
 H      -1.007257     3.006427     2.280841      23.56
 H       0.596318     2.562162     2.003543      24.89
 H      -0.360436     3.070800     0.345075      23.56
 C      -0.445601    -0.904314    -0.353838      -9.31
 O      -1.835673    -1.020094    -0.236198     134.11
 C       0.270483    -1.587151    -1.422318      78.66
 H      -0.202993    -2.422184    -2.049471      22.44
 C       2.215639    -0.001796    -0.969768      37.77
 C       3.673718     0.306779    -1.090842      87.48
 H       4.328975     0.133210    -2.142542      23.90
 O       3.793817     1.760357    -0.911604     206.71
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 H       4.631986     1.929444    -0.445188      22.24
 C       4.680622    -0.297372    -0.095699      91.64
 H       4.345680    -0.059042     0.884740      27.17
 O       4.515986    -1.720970    -0.145573     305.68
 H       4.474202    -2.190782    -1.021531      29.54
 C       6.149537     0.119309    -0.243722     104.94
 O       6.458451     1.531301     0.108031     287.42
 H       6.824308     1.576147     1.050069      26.59
 H       6.324226    -0.041280    -1.225363      31.80
 H       6.985290    -0.571554     0.147024      28.74
55
name= lig-ACN-Water-frame_368
 C      -3.702503     0.767085    -3.403291      54.37
 H      -3.626631    -0.121778    -3.912140      26.64
 C      -3.517452     2.083769    -1.354710      74.21
 H      -3.256723     2.127729    -0.362518      25.90
 C      -3.367804     3.214856    -2.148746      13.74
 O      -3.420254     4.527047    -1.609921     248.56
 C      -3.651338     4.832100    -0.211989     109.37
 H      -2.992232     4.338377     0.571643      26.52
 H      -4.777754     4.674074    -0.108813      25.82
 H      -3.444375     5.954584    -0.022125      26.08
 C      -3.411059     3.241119    -3.576798       0.85
 O      -3.312429     4.357636    -4.256582     185.32
 H      -3.333382     5.176037    -3.711784      20.82
 C      -3.335438     1.868318    -4.219344      32.51
 H      -3.431499     1.766060    -5.266510      20.65
 C      -3.744125     0.781582    -1.974725      24.55
 C      -3.896097    -0.611197    -1.286085      97.83
 H      -4.565480    -1.226668    -1.791014      27.36
 O      -4.646132    -0.421824    -0.102064     222.41
 H      -4.184065    -0.192858     0.703498      26.99
 C      -2.709838    -1.541217    -1.165963      59.88
 H      -2.273301    -1.871125    -2.320701      25.68
 C      -3.251296    -2.925963    -0.539454     106.00
 O      -3.779073    -3.652991    -1.687345     151.59
 H      -2.930114    -3.778856    -2.260737      27.03
 H      -4.037258    -2.572785     0.164700      25.99
 H      -2.321289    -3.324667     0.086783      26.15
 C       1.592382    -1.139806    -1.688775      40.08
 H       2.108562    -1.784553    -2.440676      23.63
 C       1.504974     0.539426     0.037941      83.96
 H       1.984464     1.370612     0.492447      27.33
 C       0.171256     0.247532     0.313523     -10.27
 O      -0.607031     0.884084     1.278839     188.65
 C      -0.282507     2.353207     1.512724      84.24
 H      -1.395036     2.684533     1.909788      22.10
 H       0.646927     2.478143     1.961203      24.74
 H      -0.117912     2.878439     0.324096      24.18
 C      -0.481907    -0.799617    -0.383311     -13.62
 O      -1.853255    -0.944391    -0.139261     103.33
 C       0.290442    -1.507934    -1.363675      66.22
 H      -0.167101    -2.471741    -1.962497      23.52
 C       2.212069    -0.110931    -0.990139       7.53
 C       3.733053     0.392119    -1.104940      83.51
 H       3.873786    -0.012065    -2.271978      25.05
 O       3.821197     1.790498    -0.967263     233.25
 H       4.479169     2.097776    -0.230371      20.11
 C       4.682913    -0.303145    -0.041365      83.52
 H       4.474158     0.033249     0.926357      27.63
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 O       4.519562    -1.731284    -0.103497     264.56
 H       4.653162    -1.836432    -1.065043      30.90
 C       6.197748     0.192522    -0.357053      99.88
 O       6.463366     1.540997     0.103953     257.50
 H       7.065264     1.486649     0.895470      25.72
 H       6.512687     0.161264    -1.325469      29.74
 H       6.675057    -0.495924     0.464081      26.32
55
name= lig-ACN-Water-frame_369
 C      -3.595939     0.779489    -3.456773      68.99
 H      -3.790574    -0.183803    -3.872232      36.89
 C      -3.474742     2.012929    -1.323254      71.77
 H      -3.560154     2.113952    -0.240757      25.41
 C      -3.328834     3.189288    -2.096204      -9.77
 O      -3.471165     4.500559    -1.637649     152.62
 C      -3.641933     4.824775    -0.153065     103.02
 H      -3.056191     4.128360     0.464524      26.93
 H      -4.673227     4.733337     0.222151      26.50
 H      -3.287475     6.005779    -0.182806      24.64
 C      -3.275080     3.102466    -3.550296       8.97
 O      -3.324362     4.320420    -4.328522      61.16
 H      -3.526174     5.171805    -3.750901      21.54
 C      -3.326870     1.936894    -4.181578     105.93
 H      -3.367900     1.917785    -5.268700      21.42
 C      -3.648886     0.786245    -2.019988     -27.42
 C      -4.005456    -0.620697    -1.359545      62.90
 H      -4.591360    -1.094756    -2.046317      27.07
 O      -4.677520    -0.431823    -0.036980     155.76
 H      -3.911174    -0.156802     0.573844      26.79
 C      -2.724530    -1.501825    -1.071750      66.06
 H      -1.889057    -1.410030    -1.991689      23.07
 C      -3.159999    -2.812982    -0.602274     116.97
 O      -3.726061    -3.612837    -1.638017     207.40
 H      -3.149794    -3.872822    -2.323326      30.00
 H      -4.009505    -2.837121     0.096743      24.54
 H      -2.392961    -3.571103    -0.093388      24.75
 C       1.596560    -1.158114    -1.708978      49.15
 H       2.020737    -1.626018    -2.604184      27.84
 C       1.453495     0.518214     0.049007      38.48
 H       1.893067     1.316946     0.527111      26.21
 C       0.160644     0.185859     0.357319      36.97
 O      -0.625389     0.840545     1.305042     216.24
 C      -0.298983     2.159326     1.493112     112.02
 H      -1.198134     2.821659     2.015695      25.13
 H       0.348454     2.322648     2.367734      27.40
 H       0.006671     2.757789     0.387189      26.47
 C      -0.542425    -0.674892    -0.457127      -1.47
 O      -1.795448    -0.872926    -0.053761     129.39
 C       0.265293    -1.482996    -1.337470      50.03
 H      -0.344143    -2.487187    -1.849474      21.49
 C       2.315023    -0.164504    -0.945480      19.23
 C       3.691562     0.344748    -1.115742      88.59
 H       4.295367     0.169354    -2.125017      22.70
 O       3.845104     1.881582    -1.046819     212.94
 H       4.538986     2.040380    -0.337649      20.42
 C       4.688044    -0.241500    -0.105376      93.39
 H       4.378876     0.022813     0.860922      26.88
 O       4.572541    -1.720309    -0.100992     270.39
 H       4.590182    -2.146451    -0.973945      29.98
 C       6.228451     0.158463    -0.320544      88.25
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 O       6.460485     1.572643     0.086681     291.24
 H       6.880029     1.689746     0.997585      24.30
 H       6.412728     0.057078    -1.372042      29.99
 H       7.011731    -0.652094     0.037629      28.73
55
name= lig-ACN-Water-frame_370
 C      -3.469663     0.679417    -3.470049      39.64
 H      -3.902998    -0.129888    -4.131943      17.32
 C      -3.449183     1.940568    -1.326230      64.84
 H      -3.970410     1.902327    -0.311051      23.17
 C      -3.363298     3.204520    -2.055208      16.64
 O      -3.511007     4.494025    -1.577124     247.27
 C      -3.609075     4.750235    -0.215086     122.80
 H      -2.894787     4.195096     0.370228      26.41
 H      -4.598561     4.749541     0.151389      26.97
 H      -3.160000     5.945368    -0.046924      24.00
 C      -3.162097     3.219749    -3.468251      -2.06
 O      -3.330492     4.204310    -4.361409     150.38
 H      -3.299351     5.205415    -3.842989      16.00
 C      -3.359054     1.928840    -4.217207      -1.85
 H      -3.168439     1.993240    -5.336834      22.55
 C      -3.561318     0.737205    -2.057209      36.09
 C      -4.007016    -0.484684    -1.320596     103.08
 H      -4.652319    -1.042036    -1.874919      31.34
 O      -4.730034    -0.457853    -0.077800     143.27
 H      -4.322815     0.117172     0.730390      22.80
 C      -2.698636    -1.368010    -1.020952      63.71
 H      -2.311118    -1.622429    -2.167271      26.93
 C      -3.082989    -2.883660    -0.586169     102.78
 O      -3.757398    -3.622096    -1.670048     206.41
 H      -3.023698    -3.862200    -2.245775      29.31
 H      -3.673628    -2.693250     0.295029      26.75
 H      -1.937767    -3.136472    -0.275937      25.07
 C       1.613926    -1.151415    -1.676569      64.76
 H       2.181751    -1.723856    -2.380417      25.15
 C       1.577969     0.541066     0.096262      38.58
 H       2.045258     1.230946     0.750117      22.93
 C       0.163903     0.220749     0.377090       2.52
 O      -0.659685     0.748873     1.324672     169.76
 C      -0.304226     2.181088     1.615221      85.45
 H      -1.364640     2.698723     1.770088      23.31
 H       0.543813     2.146045     2.340285      23.96
 H       0.351870     2.674563     0.599198      24.44
 C      -0.491417    -0.710266    -0.471228     -18.72
 O      -1.899412    -0.844659    -0.009014     142.68
 C       0.223716    -1.475615    -1.422162      59.82
 H      -0.254812    -2.435947    -2.151231      19.41
 C       2.229735    -0.134717    -0.901672      23.98
 C       3.787968     0.388442    -1.182531      68.80
 H       3.923685    -0.007414    -2.262679      22.09
 O       3.831297     1.870975    -1.113345     244.92
 H       4.667028     2.126064    -0.725041      20.90
 C       4.764828    -0.291668    -0.097029      91.71
 H       4.439299     0.073393     0.855181      25.28
 O       4.636348    -1.703066    -0.103084     320.05
 H       4.557037    -1.893408    -1.088609      28.03
 C       6.196236     0.154074    -0.331748     101.28
 O       6.449236     1.562087     0.052208     297.43
 H       6.683059     1.510804     1.019300      26.51
 H       6.372025     0.231896    -1.421657      31.02
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 H       6.979882    -0.423317     0.269855      28.43
55
name= lig-ACN-Water-frame_371
 c
55
name= lig-ACN-Water-frame_372
 C      -3.372362     0.624321    -3.374763      34.22
 H      -3.205022    -0.367814    -4.003369      26.01
 C      -3.592156     1.998819    -1.416696      70.22
 H      -3.452989     2.058992    -0.229779      26.11
 C      -3.383918     3.229633    -2.162814       9.17
 O      -3.503284     4.480304    -1.590335     203.02
 C      -3.562159     4.622063    -0.059066      97.68
 H      -2.685718     4.174284     0.353803      27.60
 H      -4.429930     4.409443     0.409737      27.49
 H      -3.200317     5.870563     0.022106      23.88
 C      -3.316446     3.171883    -3.569851       7.76
 O      -3.237805     4.261997    -4.309864     157.68
 H      -3.250290     5.013010    -3.691354      24.11
 C      -3.143510     1.864218    -4.204889       4.58
 H      -3.022248     1.878067    -5.363370      13.88
 C      -3.598110     0.732218    -2.004268      32.41
 C      -4.047187    -0.581169    -1.337869      69.29
 H      -4.708408    -1.134974    -1.978294      24.23
 O      -4.909504    -0.272666    -0.124691     173.11
 H      -4.421362    -0.125438     0.671075      28.05
 C      -2.661617    -1.507982    -1.042489      76.05
 H      -2.433916    -1.711241    -2.163688      28.49
 C      -2.948802    -3.005952    -0.682304     125.62
 O      -3.824927    -3.594516    -1.575793     184.42
 H      -3.184386    -3.879315    -2.389052      25.66
 H      -3.357053    -2.803278     0.276955      28.50
 H      -1.779051    -3.286506    -0.507068      26.57
 C       1.645285    -1.035444    -1.607049      53.00
 H       2.143786    -1.425615    -2.479200      15.48
 C       1.599798     0.538765     0.176179      58.23
 H       1.841639     1.393840     0.877585      24.19
 C       0.198963     0.208956     0.465729      -9.53
 O      -0.514078     0.860231     1.387078     193.51
 C      -0.308123     2.176136     1.872663     104.26
 H      -1.265965     2.564850     1.997268      25.75
 H       0.501760     1.965506     2.722984      22.77
 H       0.445816     2.917784     1.063201      23.02
 C      -0.455434    -0.781137    -0.387386      15.26
 O      -1.803697    -0.821667    -0.172828     171.64
 C       0.222788    -1.324511    -1.417643      75.33
 H      -0.211069    -2.171957    -2.168357      26.46
 C       2.253363    -0.043647    -0.853475      45.20
 C       3.733600     0.293795    -1.153550      94.86
 H       3.940062    -0.131949    -2.137454      28.28
 O       3.845845     1.774118    -1.247284     177.72
 H       4.734195     2.038279    -0.725066      17.23
 C       4.750951    -0.270501    -0.204805      86.77
 H       4.424447     0.042221     0.848509      24.58
 O       4.740960    -1.731085    -0.178018     274.54
 H       4.589725    -2.032054    -1.153864      29.36
 C       6.247308     0.104962    -0.337379      93.61
 O       6.368210     1.585169    -0.041596     259.20
 H       6.668631     1.584384     0.927045      25.14
 H       6.450803     0.177682    -1.515308      27.54
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 H       6.957376    -0.352239     0.307444      30.23
55
name= lig-ACN-Water-frame_373
 C      -3.268736     0.713509    -3.374993      35.36
 H      -3.413082    -0.336791    -3.808334      18.91
 C      -3.598352     2.027884    -1.365374      52.71
 H      -3.965737     2.165390    -0.275587      19.28
 C      -3.505081     3.150397    -2.146406     -13.30
 O      -3.475701     4.500806    -1.524210     209.72
 C      -3.476944     4.553964    -0.116602     109.59
 H      -2.666439     4.005977     0.382169      27.28
 H      -4.349043     4.130367     0.226828      26.83
 H      -3.600590     5.791636     0.184636      23.31
 C      -3.343737     3.096721    -3.632073      -2.07
 O      -3.172776     4.371107    -4.300288     126.22
 H      -3.388688     5.118347    -3.800031      22.76
 C      -3.134107     1.808605    -4.199139      68.09
 H      -2.581223     1.610084    -5.142057      26.99
 C      -3.680054     0.703918    -2.014835      10.15
 C      -4.081521    -0.611136    -1.288831      92.68
 H      -4.713322    -1.283947    -1.921880      28.55
 O      -4.911568    -0.215707    -0.189942     180.42
 H      -4.330726    -0.019062     0.634556      25.07
 C      -2.680825    -1.542509    -1.176784      87.60
 H      -2.029334    -1.444493    -2.065468      27.75
 C      -2.862910    -2.989985    -0.576319     113.77
 O      -3.861587    -3.635514    -1.577982     160.72
 H      -3.382801    -3.997896    -2.346254      29.69
 H      -3.363337    -3.245554     0.336063      27.70
 H      -2.062832    -3.822773    -0.722929      25.53
 C       1.612318    -0.952967    -1.689341      57.12
 H       2.089703    -1.400179    -2.580801      28.62
 C       1.506499     0.605561     0.217927      43.49
 H       2.196245     1.351142     0.638810      21.45
 C       0.274830     0.212890     0.516000      47.38
 O      -0.531700     0.883039     1.420195     182.40
 C      -0.209931     2.189201     2.014786     103.34
 H      -1.067134     2.633049     2.343155      27.77
 H       0.288017     2.221353     3.120548      25.35
 H       0.276991     3.039080     1.115900      24.09
 C      -0.413974    -0.629988    -0.347201       2.81
 O      -1.821832    -0.826728    -0.204336     118.64
 C       0.361159    -1.330741    -1.384751      67.63
 H      -0.245233    -2.029797    -2.035139      23.64
 C       2.317989    -0.109807    -0.804803       1.03
 C       3.721656     0.321045    -1.205100      82.46
 H       3.844053     0.042368    -2.204169      24.81
 O       3.907422     1.751920    -1.280187     209.19
 H       4.418781     2.064487    -0.454192      19.79
 C       4.798686    -0.380815    -0.138377      81.06
 H       4.410860    -0.016919     0.894298      22.44
 O       4.759437    -1.773883    -0.206479     298.78
 H       4.536728    -2.020572    -1.167000      26.27
 C       6.204297     0.180689    -0.370941      92.46
 O       6.332176     1.588314    -0.105119     322.86
 H       6.662849     1.780848     0.820924      26.32
 H       6.625256    -0.141507    -1.439764      27.78
 H       6.780448    -0.524825     0.178478      30.02
55
name= lig-ACN-Water-frame_374
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 C      -3.290597     0.665741    -3.383052      46.60
 H      -3.088855    -0.232916    -3.932474      25.46
 C      -3.733526     1.948731    -1.361094      76.32
 H      -4.059319     1.965175    -0.333241      20.92
 C      -3.596146     3.197066    -2.141391       2.55
 O      -3.437634     4.424619    -1.601262     222.62
 C      -3.478947     4.450905    -0.125708     101.52
 H      -2.480773     4.121359     0.263423      26.42
 H      -4.273704     3.915693     0.317188      24.89
 H      -3.530164     5.638352     0.218291      23.82
 C      -3.280001     3.175801    -3.543904      -0.86
 O      -3.138184     4.320729    -4.297071      52.26
 H      -3.063023     5.127308    -3.649439      23.64
 C      -3.076236     1.894113    -4.151998      16.42
 H      -2.873558     1.858386    -5.212054      18.66
 C      -3.683592     0.753940    -2.030579      35.18
 C      -3.973073    -0.601339    -1.314630      73.86
 H      -4.694264    -1.165431    -2.032055      24.15
 O      -4.862570    -0.244235    -0.185661     137.60
 H      -4.278277     0.196857     0.576360      24.68
 C      -2.716965    -1.522448    -1.118477      83.10
 H      -2.514788    -1.638244    -2.166870      28.89
 C      -2.908143    -3.035432    -0.675405     120.42
 O      -3.865938    -3.664572    -1.552029     225.62
 H      -3.313161    -3.989939    -2.242979      31.03
 H      -3.167540    -2.861492     0.373147      27.73
 H      -1.796740    -3.325221    -0.643263      26.14
 C       1.664274    -0.934766    -1.722919      45.04
 H       2.226217    -1.440512    -2.559768      24.86
 C       1.722066     0.638528     0.218649      41.54
 H       2.035496     1.379630     0.886846      21.25
 C       0.232203     0.345114     0.533456     -33.92
 O      -0.606408     0.937811     1.547395     139.53
 C      -0.151548     2.209268     2.154054      89.61
 H      -1.075136     2.667763     2.405300      24.63
 H       0.758503     1.943029     2.913561      22.08
 H       0.439145     2.896976     1.209381      22.49
 C      -0.454184    -0.662030    -0.399162       5.24
 O      -1.799404    -0.787042    -0.155039     143.73
 C       0.273797    -1.323847    -1.349072      75.20
 H      -0.157134    -2.033376    -1.996671      23.08
 C       2.336926    -0.036739    -0.861690      35.67
 C       3.767423     0.294697    -1.172796     101.11
 H       4.086477    -0.062611    -2.025991      26.10
 O       3.926523     1.769881    -1.259397     240.88
 H       4.464398     2.015074    -0.528538      23.07
 C       4.743591    -0.325730    -0.164793      85.89
 H       4.547202    -0.221192     0.980206      22.75
 O       4.757961    -1.862739    -0.230801     263.50
 H       4.793405    -2.134696    -1.192809      28.62
 C       6.208954     0.141864    -0.391089     103.06
 O       6.294099     1.596322    -0.146320     260.84
 H       6.788787     1.587465     0.711553      26.68
 H       6.461411     0.063232    -1.516873      31.11
 H       6.933335    -0.205423     0.297748      29.82
55
name= lig-ACN-Water-frame_375
 C      -3.291495     0.723253    -3.474537      86.63
 H      -3.035446    -0.165852    -3.885362      28.51
 C      -3.921626     1.991445    -1.461495      57.46
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 H      -3.921687     2.024208    -0.455948      25.98
 C      -3.576507     3.131255    -2.122799      23.35
 O      -3.453324     4.403953    -1.580933     210.07
 C      -3.436008     4.400344    -0.143854     112.03
 H      -2.431535     3.978836     0.221760      26.50
 H      -4.279591     3.851514     0.358767      25.84
 H      -3.586357     5.528851     0.070540      25.71
 C      -3.208391     3.170093    -3.439954      11.96
 O      -3.106946     4.251817    -4.249365     155.98
 H      -2.997545     5.294549    -3.882141      19.79
 C      -3.073645     1.954477    -4.099259      59.76
 H      -2.987354     2.039681    -5.138291      20.95
 C      -3.601742     0.695570    -2.110068     -29.00
 C      -3.954457    -0.532518    -1.322594      78.88
 H      -4.611746    -1.264383    -2.009533      22.73
 O      -4.758102    -0.334057    -0.140461     177.07
 H      -4.212039     0.048490     0.611042      23.82
 C      -2.746545    -1.435130    -1.071264      96.00
 H      -2.114568    -1.410504    -1.912580      27.20
 C      -2.934776    -2.890821    -0.678240     120.72
 O      -3.797570    -3.711510    -1.508756     173.72
 H      -3.345567    -4.006666    -2.400479      27.03
 H      -3.486254    -3.190164     0.234968      25.30
 H      -2.003797    -3.493404    -0.739877      25.71
 C       1.603069    -0.955337    -1.601374      49.66
 H       2.106999    -1.489538    -2.460478      17.95
 C       1.611297     0.611297     0.287764      45.15
 H       2.301606     1.151051     0.778641      22.54
 C       0.259688     0.423274     0.415504       8.27
 O      -0.571510     0.973005     1.588964     145.02
 C      -0.055008     2.166992     2.194062     100.84
 H      -0.723128     2.738374     2.915633      24.79
 H       0.711583     1.898147     3.090965      24.39
 H       0.425448     3.014964     1.380738      22.56
 C      -0.423248    -0.574559    -0.318052      -7.62
 O      -1.832447    -0.800566    -0.138827     128.70
 C       0.287938    -1.282180    -1.437562      66.61
 H      -0.160847    -2.023097    -1.884196      25.53
 C       2.301120     0.081313    -0.922062      13.82
 C       3.846284     0.302070    -1.153944      94.35
 H       4.018599    -0.024922    -2.045703      29.55
 O       3.915424     1.781527    -1.196422     213.56
 H       4.812401     2.038716    -0.902297      20.84
 C       4.806769    -0.430667    -0.130701      80.32
 H       4.347509    -0.027612     0.881348      24.28
 O       4.754778    -1.851238    -0.255104     310.48
 H       4.637949    -1.990217    -1.250101      27.89
 C       6.208223     0.122245    -0.415309     102.75
 O       6.305569     1.592615    -0.142690     270.56
 H       6.423613     1.786960     0.828610      26.22
 H       6.441480    -0.053702    -1.482987      32.20
 H       6.848774    -0.600274     0.069982      31.50
55
name= lig-ACN-Water-frame_376
 C      -3.229915     0.717094    -3.525317      43.70
 H      -3.282867    -0.095942    -4.122890      21.95
 C      -3.951742     1.930052    -1.514352     100.44
 H      -4.389362     1.851099    -0.577440      26.16
 C      -3.517477     3.174094    -2.079698       5.55
 O      -3.523853     4.410311    -1.494350     238.50
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 C      -3.390357     4.428557    -0.095178     126.24
 H      -2.447611     3.902176     0.320546      25.51
 H      -4.327360     3.874854     0.330412      24.39
 H      -3.411525     5.441169     0.304924      25.71
 C      -3.166641     3.135389    -3.500912      11.65
 O      -3.048541     4.282182    -4.241971     135.96
 H      -3.190511     5.072567    -3.478910      16.34
 C      -3.083778     1.947591    -4.193957      84.63
 H      -2.640238     1.900045    -5.155033      29.07
 C      -3.682030     0.754187    -2.127084      11.45
 C      -3.955608    -0.576435    -1.327930      82.26
 H      -4.719222    -1.234168    -2.019801      23.16
 O      -4.644302    -0.415078    -0.085499     181.72
 H      -4.074384    -0.122624     0.630459      23.82
 C      -2.607946    -1.351521    -1.141100      72.60
 H      -2.227464    -1.374271    -2.077999      28.94
 C      -2.961256    -2.886041    -0.596456     103.01
 O      -3.782961    -3.745116    -1.540759     208.00
 H      -3.075142    -3.857901    -2.347844      25.10
 H      -3.325252    -2.657463     0.444954      24.98
 H      -1.950711    -3.237263    -0.403156      25.94
 C       1.625340    -0.941465    -1.594188      59.67
 H       2.223130    -1.536504    -2.321718      17.99
 C       1.591809     0.647413     0.218640      60.17
 H       1.938447     1.242641     0.951789      25.21
 C       0.158184     0.449688     0.484353     -20.05
 O      -0.464585     0.979795     1.501773     179.92
 C       0.087483     2.140542     2.303780      83.17
 H      -0.971272     2.379109     2.735927      21.72
 H       1.045658     1.827093     2.857181      22.41
 H       0.367228     2.979785     1.467461      22.00
 C      -0.503325    -0.535045    -0.395708       6.48
 O      -1.804499    -0.762810    -0.008326     184.01
 C       0.204191    -1.191619    -1.334975      78.70
 H      -0.130614    -1.906993    -1.834894      28.31
 C       2.270981     0.052619    -0.847812      42.04
 C       3.716945     0.353603    -1.186697      94.87
 H       3.993712     0.017234    -2.048415      27.16
 O       3.941435     1.781086    -1.115167     197.31
 H       4.966165     1.924399    -1.002943      16.73
 C       4.799104    -0.401229    -0.126338      69.71
 H       4.692953    -0.339231     1.057303      21.95
 O       4.737794    -1.817192    -0.297999     319.01
 H       4.507994    -2.149262    -1.218906      28.31
 C       6.239042     0.090578    -0.420650     111.59
 O       6.354836     1.493714    -0.133068     320.47
 H       6.531996     1.590197     0.868753      24.00
 H       6.416194     0.056856    -1.460546      30.68
 H       7.116657    -0.299647     0.133286      28.70
55
name= lig-ACN-Water-frame_377
 C      -3.270189     0.665775    -3.506528      75.26
 H      -3.123952    -0.306907    -3.944324      25.42
 C      -3.913652     1.973666    -1.471104     -11.32
 H      -4.581805     2.037505    -0.606694      17.72
 C      -3.504706     3.160774    -2.147903      -6.15
 O      -3.586465     4.444386    -1.472601     158.01
 C      -3.396674     4.433663     0.073999      97.30
 H      -2.436367     3.829430     0.247020      24.91
 H      -4.292837     4.084274     0.817917      23.28
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 H      -3.239359     5.416355     0.193880      25.98
 C      -3.166081     3.162686    -3.533585     -34.18
 O      -2.981224     4.345156    -4.200781     100.55
 H      -2.891318     5.318979    -3.714156      21.26
 C      -2.999805     1.874530    -4.282127       0.82
 H      -2.731427     1.934667    -5.355096      18.21
 C      -3.792254     0.682908    -2.211928       7.79
 C      -3.897235    -0.598199    -1.378274      81.74
 H      -4.561569    -1.475802    -1.951021      24.78
 O      -4.570787    -0.484594    -0.052111     150.36
 H      -4.046757     0.162642     0.536831      22.36
 C      -2.619740    -1.442103    -1.155985      87.27
 H      -1.972821    -1.428324    -1.882846      28.51
 C      -2.914974    -2.808408    -0.576772     121.46
 O      -3.700738    -3.662460    -1.484489     250.27
 H      -3.149517    -4.112011    -2.192129      29.10
 H      -3.780940    -2.736528     0.146898      22.89
 H      -2.137746    -3.391130    -0.248916      26.78
 C       1.568959    -0.923768    -1.583304      54.05
 H       2.035249    -1.538004    -2.363175      25.18
 C       1.532750     0.752667     0.202401      67.41
 H       2.086588     1.535139     0.649460      19.90
 C       0.258917     0.386842     0.434338      27.22
 O      -0.439139     1.022770     1.505023     217.37
 C       0.133783     2.059166     2.268140     112.30
 H      -0.514261     2.401890     3.242691      23.68
 H       0.984144     1.742318     2.933671      25.32
 H       0.390081     3.028596     1.715213      24.73
 C      -0.544545    -0.409235    -0.341375      11.07
 O      -1.853803    -0.749581     0.001367     155.18
 C       0.244100    -1.212234    -1.331421      57.05
 H      -0.255280    -1.876176    -1.851940      21.85
 C       2.258659    -0.004959    -0.764486      25.01
 C       3.730515     0.370133    -1.059648     103.31
 H       3.811379     0.050087    -1.972023      25.85
 O       3.955083     1.813793    -1.076192     215.90
 H       4.751465     1.966306    -0.386431      15.80
 C       4.777787    -0.372417    -0.193234      90.22
 H       4.411227    -0.034071     0.881213      21.19
 O       4.695407    -1.841712    -0.343428     323.08
 H       4.831128    -1.930730    -1.345057      27.29
 C       6.299737     0.047142    -0.469125      90.45
 O       6.432814     1.464450    -0.114222     299.80
 H       6.876115     1.570855     0.798257      26.17
 H       6.523103    -0.124352    -1.457629      34.03
 H       6.825742    -0.731567     0.175245      30.04
55
name= lig-ACN-Water-frame_378
 C      -3.324625     0.673010    -3.552816      53.38
 H      -2.915148    -0.305888    -3.992167      24.25
 C      -3.905450     1.957067    -1.569645      81.71
 H      -3.983933     2.037331    -0.416857      21.51
 C      -3.567183     3.172501    -2.137249       4.78
 O      -3.651381     4.390356    -1.415267     208.54
 C      -3.355428     4.461646     0.062330     107.95
 H      -2.567739     3.743377     0.445000      26.54
 H      -4.446882     4.181212     0.587534      24.02
 H      -3.134122     5.368434     0.262552      28.15
 C      -3.122914     3.149008    -3.554029      10.50
 O      -2.892571     4.358036    -4.232397     131.89
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 H      -2.941070     5.050307    -3.530070      24.05
 C      -2.980969     1.887968    -4.158130      45.00
 H      -2.768837     1.792944    -5.274648      17.36
 C      -3.802182     0.706105    -2.157959     -26.50
 C      -3.911145    -0.676550    -1.371533      86.32
 H      -4.716730    -1.346137    -2.054504      22.97
 O      -4.549076    -0.512872    -0.147215     171.77
 H      -4.046819     0.069962     0.601353      20.21
 C      -2.578938    -1.432939    -1.079609     100.48
 H      -2.172593    -1.585328    -2.005110      27.55
 C      -2.984591    -2.839549    -0.511138     123.76
 O      -3.642750    -3.610985    -1.477595     295.14
 H      -3.022574    -3.915418    -2.095388      30.46
 H      -3.498701    -2.606096     0.477754      24.67
 H      -2.082784    -3.152470    -0.153589      28.15
 C       1.564597    -0.941200    -1.530285      45.09
 H       2.131539    -1.421413    -2.323971      22.72
 C       1.622509     0.836046     0.172557      56.56
 H       2.125734     1.784352     0.588887      19.61
 C       0.222096     0.515133     0.536159      -5.09
 O      -0.523369     1.042981     1.533678     192.57
 C       0.233991     2.022746     2.319942      99.33
 H      -0.622064     2.254970     3.144734      22.32
 H       1.235618     1.634975     2.444714      25.26
 H       0.390078     2.879432     1.663861      25.90
 C      -0.480205    -0.520278    -0.347331       6.57
 O      -1.883527    -0.719438    -0.077742     177.59
 C       0.168274    -1.191407    -1.321838      60.78
 H      -0.159530    -2.038723    -1.920433      22.03
 C       2.308650    -0.009124    -0.775329      36.68
 C       3.751118     0.354315    -1.091918      97.59
 H       4.000997     0.168039    -2.033802      24.85
 O       3.966773     1.848475    -1.002606     216.08
 H       4.323840     2.176448    -0.153458      21.32
 C       4.795242    -0.392120    -0.241757      99.86
 H       4.677539    -0.285070     0.923504      22.39
 O       4.652331    -1.789923    -0.400045     302.03
 H       4.757072    -2.160446    -1.324855      30.11
 C       6.227085    -0.023364    -0.454665     108.56
 O       6.588868     1.429204    -0.109671     281.85
 H       6.720463     1.499051     0.895499      26.25
 H       6.570770    -0.099076    -1.437106      31.66
 H       6.945643    -0.662116     0.179530      29.75
55
name= lig-ACN-Water-frame_379
 C      -3.344059     0.694735    -3.466160      66.66
 H      -3.350279    -0.222048    -4.242419      22.60
 C      -3.866405     1.910478    -1.536095      39.52
 H      -3.987574     1.787340    -0.335140      19.58
 C      -3.599353     3.190795    -2.155271      29.41
 O      -3.663410     4.336776    -1.411397     238.69
 C      -3.394224     4.431388    -0.046665     112.06
 H      -2.657135     3.690019     0.306491      26.97
 H      -4.429102     4.348385     0.670966      22.88
 H      -3.034587     5.330794     0.045040      27.82
 C      -3.131839     3.214553    -3.452114      11.39
 O      -2.797988     4.260002    -4.247528     202.02
 H      -2.982972     5.121146    -3.990357      23.03
 C      -3.008425     1.926701    -4.098637       7.98
 H      -2.392546     1.974245    -5.070095      23.13
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 C      -3.699728     0.638728    -2.187643      21.89
 C      -3.926184    -0.623264    -1.415359      84.56
 H      -4.513356    -1.490586    -2.118157      23.14
 O      -4.664691    -0.496356    -0.181646     152.47
 H      -3.951106    -0.120746     0.511209      22.19
 C      -2.671598    -1.448623    -1.108578      84.62
 H      -2.011379    -1.594228    -1.944123      24.30
 C      -2.900818    -2.813255    -0.371510     114.26
 O      -3.654621    -3.627225    -1.462483     204.06
 H      -3.029885    -3.737452    -2.247283      28.67
 H      -3.666478    -2.830592     0.452261      24.81
 H      -2.083656    -3.373104    -0.227526      27.79
 C       1.641903    -0.966116    -1.497916      12.75
 H       2.095279    -1.622555    -2.242033      17.68
 C       1.529182     0.834539     0.205503      57.93
 H       2.089345     1.737631     0.794667      18.01
 C       0.206156     0.513241     0.436300      15.99
 O      -0.583155     1.067444     1.548419     188.87
 C       0.269684     2.020515     2.317624     113.27
 H      -0.094348     2.184986     3.450517      24.02
 H       1.174837     1.598545     2.606073      26.37
 H       0.285670     2.937186     1.858287      26.37
 C      -0.442829    -0.536936    -0.224499      14.19
 O      -1.791260    -0.633226    -0.149633     173.47
 C       0.260270    -1.199307    -1.332439      93.09
 H      -0.377178    -2.018018    -1.923969      17.29
 C       2.301227     0.081660    -0.834979      25.69
 C       3.806012     0.437180    -1.160876      95.31
 H       4.004236     0.202748    -2.147934      26.62
 O       3.951403     1.858904    -0.937788     252.05
 H       4.261295     1.949730    -0.056663      24.95
 C       4.804506    -0.421270    -0.192379      72.70
 H       4.449943    -0.228812     0.898786      24.44
 O       4.602448    -1.826957    -0.457098     361.29
 H       4.529482    -1.846204    -1.462573      28.36
 C       6.326061     0.040287    -0.452103      96.13
 O       6.719331     1.326970    -0.129558     301.36
 H       6.845446     1.454327     0.859336      27.59
 H       6.389793    -0.129520    -1.527178      32.97
 H       6.914638    -0.773305     0.137223      29.62
55
name= lig-ACN-Water-frame_380
 C      -3.304513     0.729878    -3.576135      44.67
 H      -3.423639    -0.329871    -4.160303      23.73
 C      -3.780069     1.864814    -1.416941      59.36
 H      -4.461426     2.041012    -0.417956      19.45
 C      -3.621187     3.074633    -2.041666      -3.86
 O      -3.708305     4.371833    -1.513335     221.82
 C      -3.412987     4.404809    -0.074800     108.62
 H      -2.738615     3.612198     0.195143      27.65
 H      -4.404812     4.392271     0.683566      23.47
 H      -2.985096     5.295409     0.106924      28.39
 C      -3.157859     3.160725    -3.424821       4.05
 O      -2.690448     4.235325    -4.286174      98.85
 H      -2.810339     5.064112    -3.808171      23.61
 C      -2.985412     1.977232    -4.077440      66.96
 H      -2.649594     2.013107    -5.162690      20.45
 C      -3.663016     0.674656    -2.122631     -22.98
 C      -3.927466    -0.670169    -1.417283      70.09
 H      -4.709613    -1.330012    -2.143868      22.52
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 O      -4.778196    -0.431312    -0.209851     145.27
 H      -4.282812    -0.001860     0.526969      25.29
 C      -2.608407    -1.464625    -1.039759      92.19
 H      -2.183604    -1.655437    -2.098934      25.11
 C      -2.891633    -2.857951    -0.449410     121.12
 O      -3.673709    -3.634363    -1.376664     247.28
 H      -3.107479    -3.951808    -2.237707      26.15
 H      -3.486362    -2.758113     0.469963      25.97
 H      -1.951112    -3.109250    -0.066966      29.29
 C       1.708276    -0.964048    -1.511516      26.12
 H       2.319099    -1.549802    -2.204772      14.61
 C       1.502275     0.766819     0.141547      48.23
 H       2.092753     1.639902     0.793529      17.38
 C       0.159855     0.483290     0.482955      19.68
 O      -0.528091     1.120160     1.528513     234.17
 C       0.246656     2.002418     2.374400     121.72
 H      -0.370666     2.022467     3.341675      24.38
 H       1.229688     1.704889     2.336129      25.20
 H       0.336614     2.907964     1.956038      27.60
 C      -0.426102    -0.528606    -0.352368      26.55
 O      -1.805162    -0.551282    -0.172073     165.83
 C       0.392068    -1.220138    -1.220555      47.48
 H      -0.104334    -2.092980    -1.985947      19.10
 C       2.267768     0.164745    -0.881060      35.26
 C       3.786761     0.460657    -1.086315      99.20
 H       4.000957     0.316315    -2.120213      22.41
 O       3.967597     1.879502    -0.883143     208.32
 H       4.536140     2.221071    -0.075338      17.98
 C       4.753819    -0.360803    -0.220633      79.01
 H       4.431831    -0.189866     0.851392      24.27
 O       4.563904    -1.821586    -0.493752     372.72
 H       4.707637    -2.134840    -1.468754      29.07
 C       6.359061    -0.079399    -0.468703      95.96
 O       6.846419     1.300594    -0.141185     284.82
 H       7.091958     1.405008     0.815780      28.67
 H       6.601999    -0.093022    -1.588687      30.14
 H       7.046072    -0.894450    -0.044390      29.40
55
name= lig-ACN-Water-frame_381
 C      -3.306684     0.705244    -3.466238      64.38
 H      -2.973173    -0.186622    -4.152987      24.86
 C      -3.795632     1.889857    -1.348010      23.29
 H      -4.217565     1.642975    -0.260594      21.77
 C      -3.537513     3.149304    -2.107463       9.36
 O      -3.767941     4.398131    -1.526926     223.75
 C      -3.424430     4.415578    -0.095949     100.81
 H      -2.815512     3.616939     0.190830      29.42
 H      -4.501939     4.280474     0.412831      23.23
 H      -2.979286     5.372409     0.184247      26.39
 C      -3.084695     3.123694    -3.474207       0.89
 O      -2.652420     4.230049    -4.175795     102.13
 H      -2.695265     5.186478    -3.684458      22.17
 C      -2.997129     1.893605    -4.205550      18.19
 H      -2.886010     1.983435    -5.286280      16.09
 C      -3.632663     0.657775    -2.135624     -20.56
 C      -3.956799    -0.652273    -1.333040      80.49
 H      -4.559054    -1.449418    -2.057083      23.26
 O      -4.846788    -0.355469    -0.265109     149.99
 H      -4.329878     0.015815     0.430062      28.79
 C      -2.623106    -1.410315    -1.081915      89.30
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 H      -1.936757    -1.477145    -2.057185      24.28
 C      -2.852026    -2.829890    -0.438562     117.91
 O      -3.689430    -3.686998    -1.295484     231.95
 H      -3.066443    -4.106248    -1.949068      28.83
 H      -3.439373    -2.725390     0.460720      25.56
 H      -2.019820    -3.511009    -0.426998      24.17
 C       1.784161    -0.929819    -1.552062      27.25
 H       2.358792    -1.527410    -2.268745      19.05
 C       1.542482     0.808341     0.129822      55.59
 H       2.108460     1.744883     0.663905      18.75
 C       0.233325     0.456014     0.498601      20.78
 O      -0.497023     1.128132     1.459070     214.96
 C       0.229650     2.007002     2.405641     127.14
 H      -0.326643     1.939146     3.351123      26.73
 H       1.119027     1.648903     2.753017      27.37
 H       0.112174     2.953138     2.088675      27.93
 C      -0.475403    -0.428744    -0.397194       1.86
 O      -1.865725    -0.573508    -0.228219     165.94
 C       0.407245    -1.335504    -1.245191      77.00
 H      -0.039646    -2.429364    -1.783472      17.07
 C       2.321979     0.160497    -0.859644      34.83
 C       3.755880     0.528257    -1.033391      92.58
 H       4.042355     0.277835    -2.056808      23.27
 O       4.008202     1.972928    -0.834903     191.64
 H       4.717779     2.039557    -0.093618      16.91
 C       4.826472    -0.413278    -0.272825     101.26
 H       4.759860    -0.315185     0.804522      22.20
 O       4.526405    -1.759769    -0.457817     369.96
 H       4.781065    -1.921024    -1.434046      25.98
 C       6.321739    -0.125219    -0.529501      82.21
 O       6.940333     1.223600    -0.142155     249.52
 H       6.793834     1.372244     0.847440      30.43
 H       6.516064    -0.312273    -1.680786      28.93
 H       6.813062    -0.902072     0.137745      29.66
55
name= lig-ACN-Water-frame_382
 C      -3.230319     0.647939    -3.451089      32.74
 H      -3.243450    -0.396974    -3.810772      21.52
 C      -3.775741     1.965203    -1.531919      71.50
 H      -3.866125     2.224314    -0.458528      19.20
 C      -3.485011     3.119467    -2.141543      11.16
 O      -3.748345     4.400639    -1.533497     240.21
 C      -3.516377     4.436870    -0.108681     105.36
 H      -2.733447     3.772459     0.137432      28.18
 H      -4.378223     4.327845     0.645408      23.60
 H      -3.135516     5.517234    -0.009555      23.84
 C      -3.014617     3.089464    -3.484198       3.68
 O      -2.624517     4.282888    -4.068174     158.78
 H      -2.943715     5.078334    -3.405502      15.76
 C      -3.086291     1.836110    -4.217068      66.87
 H      -2.652753     1.658215    -5.158572      28.20
 C      -3.659191     0.690202    -2.075717      48.46
 C      -3.956620    -0.604013    -1.415627      82.82
 H      -4.641610    -1.337859    -2.099166      24.32
 O      -4.863135    -0.314004    -0.255683     156.62
 H      -4.352441    -0.070068     0.617637      22.98
 C      -2.669509    -1.414907    -1.121415      70.76
 H      -2.260281    -1.556202    -2.276079      21.89
 C      -2.798858    -2.817537    -0.441925     101.98
 O      -3.740553    -3.745667    -1.242568     212.78
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 H      -3.301354    -4.077210    -1.993193      31.03
 H      -3.172862    -2.767201     0.590335      25.61
 H      -1.681516    -3.029437    -0.228961      23.73
 C       1.680208    -0.966659    -1.543988      21.56
 H       2.259986    -1.588867    -2.220822      21.99
 C       1.609224     0.905596     0.186450      61.40
 H       2.030286     1.805493     0.768799      17.58
 C       0.280471     0.480025     0.366648       7.76
 O      -0.484286     1.121368     1.414066     192.92
 C       0.127802     1.987552     2.474925     116.41
 H      -0.502468     1.927362     3.269743      25.79
 H       1.154359     1.702801     2.515547      24.99
 H       0.344729     2.977959     2.094730      25.32
 C      -0.397126    -0.511928    -0.435151      18.95
 O      -1.812950    -0.571487    -0.204059     149.21
 C       0.370550    -1.268961    -1.267260      44.54
 H      -0.161696    -2.362707    -1.643666      15.81
 C       2.387143     0.132020    -0.820293      37.35
 C       3.878383     0.583340    -1.079503      75.13
 H       3.994054     0.524646    -2.185164      21.49
 O       4.068862     1.989318    -0.778264     219.01
 H       4.527497     2.218663     0.019426      22.67
 C       4.846032    -0.319473    -0.194325     103.35
 H       4.625828    -0.083838     0.807451      23.78
 O       4.510893    -1.746590    -0.445949     372.84
 H       4.470038    -2.016561    -1.398690      28.82
 C       6.361409    -0.134315    -0.539723     100.59
 O       6.923113     1.072957    -0.175257     273.71
 H       6.891396     1.282833     0.808018      31.07
 H       6.689756    -0.283550    -1.703022      28.39
 H       6.930508    -0.997706    -0.073294      29.03
55
name= lig-ACN-Water-frame_383
 C      -3.272353     0.592022    -3.463522      75.56
 H      -3.276182    -0.211640    -4.083327      24.88
 C      -3.770272     1.972205    -1.482079      58.57
 H      -4.261109     1.915969    -0.568075      21.06
 C      -3.482158     3.187233    -2.214264      -4.81
 O      -3.698362     4.355022    -1.599840     216.01
 C      -3.528364     4.520754    -0.100307      97.57
 H      -2.683274     3.984897     0.329765      27.06
 H      -4.453345     4.160837     0.312940      23.80
 H      -3.467777     5.707309     0.183822      22.53
 C      -3.004526     3.086808    -3.567784       6.72
 O      -2.603930     4.319597    -4.024019     142.66
 H      -2.801911     5.052091    -3.433107      19.47
 C      -3.011922     1.809587    -4.140157      54.77
 H      -2.706403     1.854463    -5.137898      22.76
 C      -3.651967     0.746042    -2.129333      33.17
 C      -4.024422    -0.556534    -1.364256      89.81
 H      -4.704496    -1.100029    -2.141705      24.66
 O      -4.834395    -0.329633    -0.223222     184.68
 H      -4.207182     0.016943     0.543141      23.12
 C      -2.710776    -1.413524    -1.103392      60.75
 H      -2.058416    -1.579694    -2.135447      21.62
 C      -2.805503    -2.794937    -0.483590     114.86
 O      -3.696020    -3.748756    -1.140835     186.45
 H      -3.285368    -3.864112    -2.074876      29.94
 H      -3.299011    -2.671343     0.515543      25.00
 H      -1.793289    -3.414826    -0.558887      23.25
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 C       1.746044    -0.895486    -1.460017      45.69
 H       2.232440    -1.537167    -2.179175      19.63
 C       1.662624     0.858894     0.143393      81.24
 H       2.138021     1.662923     0.664573      18.08
 C       0.271027     0.635774     0.359609      18.36
 O      -0.525024     1.103178     1.364036     213.71
 C       0.093015     1.918875     2.396323     121.57
 H      -0.520840     1.876301     3.173924      27.70
 H       0.924824     1.452719     2.883754      25.81
 H       0.006641     3.006826     2.110548      23.61
 C      -0.388505    -0.492369    -0.351288      21.55
 O      -1.745535    -0.613392    -0.210167     169.97
 C       0.306561    -1.219627    -1.323259     100.21
 H      -0.112082    -2.058950    -2.119941      17.37
 C       2.408994     0.119314    -0.840743      28.67
 C       3.903077     0.575741    -1.079813      82.41
 H       4.340928     0.462853    -2.133560      22.46
 O       4.128086     1.992992    -0.759165     209.60
 H       4.161717     2.210931     0.170951      24.16
 C       4.848527    -0.300074    -0.252979     106.34
 H       4.666695    -0.090410     0.732336      27.24
 O       4.490546    -1.710496    -0.386608     356.37
 H       4.708196    -1.854295    -1.323992      29.91
 C       6.400864    -0.276601    -0.536655      86.51
 O       6.944385     1.062348    -0.182237     234.50
 H       7.100005     1.055039     0.790538      30.71
 H       6.267745    -0.204794    -1.746439      29.57
 H       6.983064    -1.141139    -0.163927      31.20
55
name= lig-ACN-Water-frame_384
 C      -3.345804     0.680062    -3.546872      59.38
 H      -3.244687    -0.221434    -3.929928      24.54
 C      -3.820781     1.946177    -1.441382      79.98
 H      -4.274257     2.045447    -0.542406      23.09
 C      -3.522273     3.086234    -2.125865      17.49
 O      -3.597591     4.470557    -1.618560     213.66
 C      -3.607628     4.551531    -0.172374     108.92
 H      -2.628552     4.158081     0.251875      26.19
 H      -4.373545     4.080973     0.316690      27.35
 H      -3.709975     5.789800    -0.045635      23.89
 C      -3.045586     3.158902    -3.454702      -4.48
 O      -2.558224     4.305460    -4.135659     180.02
 H      -2.590509     5.040313    -3.571047      24.57
 C      -2.842876     1.891757    -4.210011      28.51
 H      -2.717663     1.755977    -5.262107      19.68
 C      -3.680039     0.672502    -2.142825       5.24
 C      -4.008281    -0.550358    -1.343094      86.69
 H      -4.590689    -1.347109    -1.869765      24.99
 O      -4.785809    -0.350404    -0.120034     177.04
 H      -4.291858     0.126143     0.541575      26.55
 C      -2.633140    -1.362094    -1.114574      62.65
 H      -2.214321    -1.308719    -2.271662      23.15
 C      -2.835077    -2.812839    -0.449462     102.34
 O      -3.690245    -3.733519    -1.124474     191.53
 H      -3.241444    -4.047595    -2.041977      26.51
 H      -3.067925    -2.748140     0.693406      24.33
 H      -1.641480    -3.130984    -0.321113      23.60
 C       1.778865    -0.926884    -1.529128      -3.18
 H       2.356670    -1.396508    -2.303528      17.64
 C       1.625427     0.888710     0.156965      74.00
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 H       2.149487     1.625903     0.673615      18.42
 C       0.268687     0.565648     0.326451      19.21
 O      -0.575569     1.126018     1.335102     217.24
 C      -0.033725     1.860114     2.402156     122.41
 H      -0.710245     1.906407     3.088710      26.70
 H       0.971532     1.477778     2.643841      24.99
 H       0.428598     2.906946     2.037020      22.80
 C      -0.399583    -0.415258    -0.412606      15.62
 O      -1.809160    -0.651045    -0.165814     179.48
 C       0.431272    -1.082051    -1.365618      52.48
 H      -0.159825    -1.758897    -2.082113      19.25
 C       2.454305     0.175760    -0.860946      25.65
 C       3.913417     0.557741    -1.033132      80.36
 H       3.938468     0.376407    -2.197474      19.51
 O       4.132835     1.958953    -0.818088     223.57
 H       4.391422     2.232910     0.167119      22.31
 C       4.903535    -0.392479    -0.179877      92.33
 H       4.855247    -0.143445     0.819629      26.66
 O       4.467924    -1.706965    -0.355924     351.59
 H       4.682828    -2.100549    -1.230937      33.90
 C       6.345061    -0.241564    -0.612829     104.98
 O       7.008330     1.013130    -0.197797     193.04
 H       6.937823     1.152390     0.782104      32.71
 H       6.745347    -0.467485    -1.725013      28.62
 H       6.806494    -1.086497    -0.065321      30.02
55
name= lig-ACN-Water-frame_385
 C      -3.331445     0.799727    -3.536002      67.93
 H      -3.325996    -0.010968    -4.151385      26.56
 C      -3.898939     1.912685    -1.456606      45.65
 H      -3.936746     1.868739    -0.405488      23.96
 C      -3.500151     3.198533    -2.104170      -7.56
 O      -3.519325     4.498978    -1.633258     195.62
 C      -3.652059     4.605191    -0.222033     117.47
 H      -2.641239     4.261197     0.230636      24.76
 H      -4.417404     4.105424     0.164755      26.83
 H      -3.691324     5.810267     0.219787      23.21
 C      -2.952808     3.127016    -3.494014      -1.12
 O      -2.544034     4.240907    -4.227639     148.10
 H      -2.585920     5.219808    -3.837044      19.19
 C      -2.895715     1.967685    -4.156210      73.95
 H      -2.295501     2.109055    -5.079423      23.90
 C      -3.801200     0.718912    -2.162162      13.89
 C      -3.939814    -0.669972    -1.300399      78.04
 H      -4.597882    -1.263558    -1.875232      26.74
 O      -4.720937    -0.374191    -0.016768     168.00
 H      -4.162874     0.159210     0.565327      27.29
 C      -2.639660    -1.357761    -1.070047      97.89
 H      -2.022154    -1.636559    -2.057024      24.01
 C      -2.740435    -2.748921    -0.408775      88.74
 O      -3.690538    -3.728166    -1.163505     162.28
 H      -3.122960    -4.192699    -1.781845      30.54
 H      -3.415811    -2.544435     0.549668      23.89
 H      -1.628437    -3.297163    -0.363800      22.75
 C       1.877296    -0.792659    -1.634403      28.24
 H       2.317151    -1.449235    -2.364524      19.21
 C       1.589194     0.915555     0.161878      66.73
 H       1.902904     1.726488     0.791890      22.31
 C       0.231360     0.525808     0.413818      -3.63
 O      -0.654041     1.129855     1.255294     175.42
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 C      -0.024275     1.877594     2.433906     104.95
 H      -0.713828     2.047662     3.126500      27.69
 H       0.633179     1.143671     2.937727      25.70
 H       0.253516     2.986910     2.045765      22.89
 C      -0.430500    -0.382084    -0.574240       4.88
 O      -1.770304    -0.632122    -0.134660     167.76
 C       0.407301    -1.028917    -1.458508      68.78
 H       0.062716    -1.891003    -1.991562      22.55
 C       2.387758     0.182627    -0.778659      33.44
 C       3.885433     0.497972    -0.985862      91.72
 H       4.399250     0.294320    -2.050078      22.15
 O       4.113230     1.940381    -0.896344     229.53
 H       4.554127     2.284305     0.002805      22.10
 C       4.885661    -0.353376    -0.211284      98.57
 H       4.805808    -0.188188     0.812987      25.49
 O       4.446749    -1.821419    -0.309155     307.58
 H       4.548198    -1.895232    -1.324839      25.55
 C       6.443974    -0.241251    -0.582727      97.43
 O       7.063162     0.970524    -0.226107     234.10
 H       6.672782     1.258494     0.642239      32.93
 H       6.485537    -0.323055    -1.758645      28.70
 H       6.954776    -1.063484    -0.059435      29.64
55
name= lig-ACN-Water-frame_386
 C      -3.366089     0.731942    -3.501493      45.55
 H      -3.281342    -0.196065    -4.103167      23.40
 C      -3.855442     2.071091    -1.507922      36.75
 H      -4.140555     2.093977    -0.403332      21.10
 C      -3.446002     3.230997    -2.192733      27.76
 O      -3.476542     4.529696    -1.637526     229.06
 C      -3.636488     4.651485    -0.162831     109.39
 H      -2.861220     4.104102     0.545786      24.36
 H      -4.496315     4.217047     0.058304      27.67
 H      -3.810840     5.859118    -0.072565      23.61
 C      -2.931651     3.249807    -3.425443      17.88
 O      -2.518572     4.230776    -4.308893     184.52
 H      -2.690834     5.167780    -3.765453      17.51
 C      -2.937792     1.975451    -4.093330      18.22
 H      -2.510815     1.754128    -5.155583      24.96
 C      -3.867087     0.747028    -2.174426      -5.18
 C      -4.008001    -0.596037    -1.292053      86.81
 H      -4.547949    -1.335978    -1.730833      27.43
 O      -4.602297    -0.439821    -0.002796     237.46
 H      -3.960990     0.006347     0.717216      21.72
 C      -2.561989    -1.435594    -1.060453      75.94
 H      -2.124704    -1.400045    -2.115107      23.66
 C      -2.828412    -2.783871    -0.396653     107.85
 O      -3.593631    -3.672318    -1.169723     247.34
 H      -3.096016    -4.059305    -1.880788      30.30
 H      -3.208175    -2.731862     0.753398      22.78
 H      -1.709276    -3.270187    -0.145965      22.78
 C       1.706206    -0.640415    -1.641668      68.83
 H       2.478759    -1.103479    -2.248711      20.30
 C       1.523018     0.886217     0.213739      59.24
 H       2.113769     1.669567     0.767497      20.65
 C       0.186313     0.548227     0.320600      26.65
 O      -0.701545     1.193173     1.290973     189.57
 C      -0.097511     1.850061     2.434018     113.79
 H      -0.929139     2.123298     2.957252      26.10
 H       0.705991     1.265013     2.985528      24.65
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 H       0.627542     2.807312     2.153034      23.01
 C      -0.388984    -0.353165    -0.544115       9.64
 O      -1.683634    -0.601468    -0.198784     167.44
 C       0.402029    -1.081884    -1.617829      42.00
 H       0.048218    -1.829788    -2.156650      21.44
 C       2.409582     0.211371    -0.753985      27.68
 C       3.910790     0.491604    -1.000793      75.29
 H       3.784973     0.173161    -2.170562      23.24
 O       4.099234     1.954945    -0.937428     226.90
 H       4.229663     2.163654    -0.003300      25.52
 C       4.898368    -0.440506    -0.109813      97.49
 H       4.725484    -0.158284     0.896025      25.47
 O       4.485250    -1.823397    -0.309908     314.68
 H       4.542463    -2.144560    -1.257349      29.18
 C       6.416814    -0.322845    -0.568607      94.78
 O       7.101031     1.010078    -0.219171     159.26
 H       6.961878     1.270595     0.740988      30.06
 H       6.472183    -0.310853    -1.684935      29.70
 H       6.987330    -1.254070    -0.325626      30.26
55
name= lig-ACN-Water-frame_387
 C      -3.434798     0.705846    -3.420283      60.84
 H      -3.280025    -0.366017    -3.896793      23.15
 C      -3.831678     2.105584    -1.552271      67.27
 H      -4.471482     2.375985    -0.592703      22.42
 C      -3.404584     3.325919    -2.147778      -3.93
 O      -3.415367     4.586159    -1.555108     198.49
 C      -3.709132     4.678248    -0.165573     120.52
 H      -2.806639     4.094041     0.348163      23.57
 H      -4.645887     4.510603     0.222684      27.68
 H      -3.424928     5.756653     0.154826      24.74
 C      -2.927459     3.160972    -3.603960     -14.84
 O      -2.499360     4.317515    -4.327200     147.72
 H      -2.378284     5.244214    -3.905414      22.10
 C      -2.956940     1.841908    -4.095723      53.88
 H      -2.861364     1.946036    -5.266893      19.84
 C      -3.830333     0.803699    -2.064742      32.81
 C      -3.959901    -0.529830    -1.289416      98.19
 H      -4.607433    -1.055384    -1.831887      27.37
 O      -4.535653    -0.488168     0.022366     234.62
 H      -3.904355     0.075834     0.693479      20.80
 C      -2.592727    -1.318541    -1.138502      85.64
 H      -2.144345    -1.710757    -2.052564      25.17
 C      -2.777749    -2.822193    -0.318479      83.72
 O      -3.550910    -3.670528    -1.211870     190.86
 H      -2.952035    -3.754833    -2.082625      27.71
 H      -3.527122    -2.595026     0.573709      21.43
 H      -1.634693    -3.204403    -0.189372      22.52
 C       1.703769    -0.599630    -1.691291      30.87
 H       2.087738    -0.948722    -2.655403      16.50
 C       1.610325     0.876118     0.271885      65.44
 H       1.936007     1.584386     1.115039      18.23
 C       0.194031     0.692595     0.282862       1.24
 O      -0.682337     1.217817     1.270485     189.82
 C      -0.130286     1.852506     2.446418     107.05
 H      -0.820506     2.329458     3.038413      26.22
 H       0.264360     0.996912     3.088353      23.88
 H       0.525852     2.804088     2.087151      21.99
 C      -0.370152    -0.472588    -0.576198      16.37
 O      -1.701448    -0.624530    -0.301337     195.31
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 C       0.307282    -0.988771    -1.582713      61.62
 H      -0.067259    -1.486111    -2.287603      23.07
 C       2.308257     0.256158    -0.725719      47.00
 C       3.806903     0.497541    -0.993466      64.71
 H       4.321580     0.322547    -2.121169      23.71
 O       4.119195     1.931751    -0.939360     213.10
 H       4.278392     2.256515    -0.054688      26.46
 C       4.899700    -0.472892    -0.118355      83.47
 H       4.902679    -0.341974     0.967280      24.55
 O       4.531543    -1.823099    -0.291730     320.18
 H       4.776968    -1.967947    -1.225094      28.68
 C       6.381299    -0.269759    -0.554637     103.40
 O       7.067759     0.951121    -0.199785     231.52
 H       7.128439     0.978732     0.779265      30.17
 H       6.410705    -0.334334    -1.616968      32.16
 H       6.969982    -1.040940     0.003284      28.88
55
name= lig-ACN-Water-frame_388
 C      -3.418123     0.733989    -3.349627      37.64
 H      -3.528884    -0.354890    -3.914882      21.40
 C      -3.895759     2.216255    -1.470555      45.36
 H      -4.238332     2.157045    -0.322362      19.47
 C      -3.342285     3.320322    -2.241762      11.42
 O      -3.378878     4.623255    -1.570513     179.80
 C      -3.667443     4.712868    -0.083896     111.40
 H      -3.293541     3.803218     0.582749      24.36
 H      -4.696582     4.500373    -0.081934      27.78
 H      -3.422262     5.727913     0.185497      25.48
 C      -2.942359     3.206980    -3.574943       3.95
 O      -2.496183     4.284505    -4.352183     200.09
 H      -2.411890     4.965844    -3.748464      26.55
 C      -3.041784     1.833997    -4.209148      29.03
 H      -2.657725     1.476347    -5.270151      21.57
 C      -3.699185     0.872994    -1.989570       8.40
 C      -3.910916    -0.510891    -1.271011      94.27
 H      -4.497055    -1.086070    -1.828320      27.87
 O      -4.539019    -0.484393     0.062757     205.04
 H      -4.116233     0.210013     0.673285      23.34
 C      -2.644909    -1.432453    -1.175798      97.50
 H      -2.276757    -1.448951    -2.158586      26.26
 C      -2.794566    -2.664601    -0.418780     111.19
 O      -3.503817    -3.689872    -1.259767     197.22
 H      -2.934582    -4.043873    -2.093743      24.30
 H      -3.355581    -2.645648     0.589764      23.43
 H      -1.803599    -3.137220    -0.008601      24.24
 C       1.678980    -0.579307    -1.762220       7.45
 H       2.330229    -0.811067    -2.619177      16.95
 C       1.584291     0.869959     0.336224      69.65
 H       2.264979     1.436075     1.049778      18.47
 C       0.199377     0.655741     0.339749      20.29
 O      -0.688208     1.235292     1.194115     199.14
 C      -0.146451     1.857952     2.461465     100.04
 H      -1.048141     2.299148     2.753535      24.64
 H       0.333270     1.094193     3.164102      24.16
 H       0.784124     2.556144     2.296942      22.07
 C      -0.433248    -0.308193    -0.457438       8.04
 O      -1.779183    -0.584225    -0.337196     156.30
 C       0.340230    -0.882337    -1.617892      68.14
 H      -0.138257    -1.484236    -2.248845      22.28
 C       2.345441     0.240062    -0.832197      22.67
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 C       3.840852     0.500590    -0.902328      83.86
 H       3.875142     0.021211    -2.082632      21.59
 O       4.158250     1.942667    -0.905644     169.90
 H       4.566830     2.153657     0.037596      23.17
 C       4.833601    -0.349804    -0.128942      88.01
 H       4.640308    -0.111079     0.951795      24.10
 O       4.589885    -1.861159    -0.313469     287.44
 H       4.586283    -2.056223    -1.286760      26.69
 C       6.364238    -0.269842    -0.524132     107.51
 O       7.017923     0.932842    -0.170639     253.27
 H       6.951833     1.164689     0.800867      30.43
 H       6.534055    -0.394422    -1.521241      32.62
 H       6.786311    -1.231196    -0.130616      30.90
55
name= lig-ACN-Water-frame_389
 C      -3.369070     0.839079    -3.361524      49.15
 H      -3.461551    -0.279866    -3.853610      22.65
 C      -3.803708     2.200448    -1.417226      68.02
 H      -3.877981     2.574869    -0.334035      18.67
 C      -3.425232     3.314259    -2.151204      -0.34
 O      -3.287080     4.612301    -1.626806     157.88
 C      -3.708502     4.669247    -0.124516     120.56
 H      -3.174305     3.934339     0.588765      24.29
 H      -4.805908     4.827009     0.041312      27.01
 H      -3.344619     5.547423     0.176369      27.49
 C      -2.977645     3.139171    -3.588049      14.05
 O      -2.497264     4.188418    -4.339834     185.60
 H      -2.513743     5.100812    -4.070664      22.62
 C      -3.109652     1.920315    -4.167947      93.73
 H      -2.706813     1.810674    -5.228954      27.42
 C      -3.641693     0.906595    -1.954058      16.58
 C      -3.973322    -0.505770    -1.223676      85.56
 H      -4.706451    -0.936725    -1.750651      27.30
 O      -4.602565    -0.442760     0.062190     208.25
 H      -4.073923     0.149970     0.597622      27.09
 C      -2.624986    -1.310764    -1.238931      99.73
 H      -2.229693    -1.564071    -2.161265      26.23
 C      -2.828574    -2.719469    -0.529396     115.39
 O      -3.461645    -3.704732    -1.265810     232.41
 H      -2.800394    -4.149629    -1.795906      28.98
 H      -3.496637    -2.422049     0.291333      24.61
 H      -1.747709    -2.964711    -0.311533      24.00
 C       1.698886    -0.481218    -1.763323      48.18
 H       2.156620    -1.180462    -2.485550      21.08
 C       1.622581     0.766376     0.232656      70.04
 H       2.057753     1.481538     0.922420      19.27
 C       0.225240     0.552146     0.449498       4.96
 O      -0.667208     1.322699     1.238947     199.74
 C      -0.190929     1.839886     2.430920     127.50
 H      -0.885313     2.503212     2.931487      25.64
 H      -0.062690     1.014526     3.186052      25.55
 H       0.575257     2.628019     2.223452      24.11
 C      -0.432880    -0.239130    -0.617474       6.69
 O      -1.817206    -0.470586    -0.279366     134.86
 C       0.294406    -0.776190    -1.581753      69.04
 H      -0.144392    -1.574702    -2.176738      21.45
 C       2.357147     0.270016    -0.750488      43.56
 C       3.849786     0.498109    -1.011522      63.62
 H       4.261124     0.476065    -2.213108      21.46
 O       4.212504     1.926007    -0.865320     214.76
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 H       4.421936     2.320921     0.120386      21.11
 C       4.808805    -0.395281    -0.125158      95.24
 H       4.686599    -0.189305     1.010953      22.61
 O       4.592196    -1.807982    -0.312743     284.88
 H       4.684942    -1.902719    -1.344968      24.78
 C       6.288772    -0.309929    -0.501231     109.52
 O       7.005043     0.995217    -0.123489     201.78
 H       6.932683     1.063197     0.888960      28.89
 H       6.310927    -0.335087    -1.493404      34.91
 H       6.840558    -1.082406     0.051618      30.31
55
name= lig-ACN-Water-frame_390
 C      -3.378823     0.808033    -3.330594      40.64
 H      -3.195013    -0.216522    -3.893246      23.51
 C      -3.625391     2.146295    -1.341281      46.19
 H      -4.065581     1.994267    -0.362972      22.00
 C      -3.439008     3.351073    -2.167860      23.92
 O      -3.247108     4.565776    -1.570039     240.15
 C      -3.676529     4.741916    -0.255017     126.03
 H      -3.253188     3.871243     0.263398      25.60
 H      -4.806199     4.453017    -0.085884      25.64
 H      -3.302600     5.597039     0.066730      28.51
 C      -3.078340     3.235513    -3.472169      13.70
 O      -2.486128     4.136643    -4.361603      90.73
 H      -2.565065     5.053739    -3.829098      22.01
 C      -3.102428     1.973125    -4.113085      42.13
 H      -3.101019     2.003402    -5.187102      22.50
 C      -3.716596     0.895894    -1.966901      24.85
 C      -4.045573    -0.404457    -1.313694      96.38
 H      -4.617805    -1.001701    -1.949520      26.60
 O      -4.663340    -0.365841     0.050849     209.37
 H      -4.142437     0.008241     0.795837      23.39
 C      -2.667944    -1.189351    -1.212381      83.55
 H      -2.212548    -1.021434    -2.123848      27.92
 C      -2.752525    -2.650851    -0.526106     113.51
 O      -3.442348    -3.768804    -1.307222     245.60
 H      -2.982397    -4.120514    -2.060761      28.61
 H      -3.299975    -2.623455     0.375921      25.63
 H      -1.843881    -3.078081    -0.118159      26.09
 C       1.662239    -0.527034    -1.722902      -0.87
 H       2.244231    -0.955088    -2.549037      22.01
 C       1.604148     0.819634     0.340906      50.57
 H       1.987852     1.519698     1.003924      20.77
 C       0.201362     0.527248     0.394172      18.27
 O      -0.656852     1.344714     1.218972     178.87
 C      -0.187177     1.910722     2.535047     118.12
 H      -1.068065     2.530182     2.808821      24.55
 H       0.099743     1.100184     3.222044      26.40
 H       0.768611     2.376422     2.480448      25.11
 C      -0.517844    -0.171061    -0.551636      14.20
 O      -1.805383    -0.398963    -0.304360     165.20
 C       0.281505    -0.763055    -1.641221      71.17
 H      -0.077673    -1.475697    -2.523227      19.73
 C       2.437629     0.234125    -0.868671       9.50
 C       3.931640     0.584205    -1.037775      76.13
 H       4.127529     0.143257    -2.175886      23.68
 O       4.249458     1.944513    -0.846563     238.73
 H       4.056282     2.168980     0.105703      24.48
 C       4.832523    -0.428051    -0.123873      86.10
 H       4.523446    -0.212505     1.007694      25.16
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 O       4.508132    -1.793646    -0.338042     289.66
 H       4.792910    -2.069152    -1.318080      27.95
 C       6.328529    -0.183455    -0.435492     120.42
 O       6.946234     0.996507    -0.132067     245.90
 H       7.077646     1.128993     0.850662      28.08
 H       6.511588    -0.347172    -1.416884      34.08
 H       6.842197    -1.080505    -0.052319      31.59
55
name= lig-ACN-Water-frame_391
 C      -3.396187     0.771408    -3.387902      68.53
 H      -3.490803    -0.190912    -3.923735      21.85
 C      -3.613690     2.118076    -1.317389      64.74
 H      -3.870906     2.308503    -0.347911      22.45
 C      -3.363489     3.283695    -2.039798     -11.47
 O      -3.202421     4.617116    -1.601720     203.69
 C      -3.652544     4.728227    -0.219238     131.70
 H      -3.164775     4.188963     0.527827      26.34
 H      -4.827495     4.647204    -0.314432      26.69
 H      -3.686123     5.766855    -0.005993      27.73
 C      -3.107027     3.245870    -3.505964      -1.27
 O      -2.521279     4.209265    -4.314873      81.47
 H      -2.275124     5.239405    -4.003182      19.10
 C      -3.154935     1.930623    -4.057556      52.09
 H      -2.847628     1.788846    -5.036874      24.83
 C      -3.771170     0.894025    -2.069099      30.86
 C      -4.048408    -0.400371    -1.251447      96.77
 H      -4.748689    -1.003528    -1.814347      25.43
 O      -4.763367    -0.282994    -0.035203     240.12
 H      -4.008432     0.118824     0.537673      25.17
 C      -2.686256    -1.163919    -1.158939      99.33
 H      -2.339956    -1.403780    -2.139243      27.06
 C      -2.702860    -2.631349    -0.546796     117.88
 O      -3.404320    -3.701146    -1.273353     229.50
 H      -2.815997    -3.888638    -2.080923      27.89
 H      -3.233054    -2.521957     0.324637      27.30
 H      -1.667360    -2.771988    -0.525755      27.08
 C       1.685687    -0.584440    -1.726345      61.04
 H       2.086008    -0.889171    -2.673099      18.46
 C       1.656880     0.825735     0.275786      68.04
 H       2.178781     1.349511     0.980494      21.70
 C       0.234044     0.708864     0.371344       3.02
 O      -0.616100     1.357085     1.257714     182.60
 C      -0.125046     1.910015     2.587903     111.89
 H      -0.988131     2.656907     2.849756      24.05
 H      -0.207168     1.165312     3.345114      25.93
 H       0.600266     2.606275     2.511703      25.93
 C      -0.444006    -0.254520    -0.577306       3.58
 O      -1.887338    -0.339139    -0.311026     161.61
 C       0.251421    -0.757319    -1.649223      58.08
 H      -0.556684    -1.335308    -2.441084      20.60
 C       2.350965     0.322613    -0.754088      25.85
 C       3.912956     0.509893    -0.971218      78.81
 H       4.193120     0.510335    -2.132209      23.46
 O       4.259273     1.972441    -0.872439     192.15
 H       4.455429     2.325328    -0.008189      26.08
 C       4.824873    -0.341824    -0.168545      74.51
 H       4.654811    -0.116421     1.024522      23.08
 O       4.425453    -1.818301    -0.357985     263.54
 H       4.450201    -1.912459    -1.404619      26.29
 C       6.393500    -0.258946    -0.432110     106.18
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 O       6.932925     1.103737    -0.134446     208.57
 H       6.713977     1.328463     0.806918      30.08
 H       6.461648    -0.322138    -1.447996      32.85
 H       6.916849    -0.987850     0.170213      31.12
55
name= lig-ACN-Water-frame_392
 C      -3.532977     0.748769    -3.425583      42.13
 H      -3.663367    -0.152006    -3.941257      25.36
 C      -3.702255     2.149168    -1.376382      37.35
 H      -3.603292     2.088657    -0.367846      29.18
 C      -3.208795     3.313658    -2.119659      11.37
 O      -3.137938     4.614194    -1.566507     148.77
 C      -3.741564     4.844097    -0.154679     113.92
 H      -3.071018     4.417849     0.472850      26.99
 H      -4.686350     4.173306     0.102823      24.31
 H      -3.563843     5.943428     0.020725      25.42
 C      -3.034914     3.162921    -3.506128       9.49
 O      -2.584913     4.263105    -4.272048     126.86
 H      -2.667511     5.112181    -3.669403      23.64
 C      -3.119285     1.958185    -4.185268      78.52
 H      -2.684523     2.011103    -5.124700      24.32
 C      -3.804289     0.846546    -1.963282     -45.41
 C      -4.090986    -0.472065    -1.297023      85.92
 H      -4.725755    -1.144897    -1.953238      23.46
 O      -4.818390    -0.168181    -0.064233     141.83
 H      -4.447406     0.374094     0.713631      24.53
 C      -2.749114    -1.241483    -1.163670      86.02
 H      -2.327678    -1.139536    -2.177833      28.74
 C      -2.643809    -2.591429    -0.492768     141.79
 O      -3.350340    -3.540509    -1.229324     228.63
 H      -2.801821    -4.157526    -1.905955      24.37
 H      -2.854554    -2.644875     0.512710      28.93
 H      -1.643555    -2.898814    -0.466656      27.65
 C       1.630695    -0.521745    -1.733119      32.76
 H       2.269334    -1.059097    -2.405079      21.30
 C       1.645128     0.908634     0.286314      63.60
 H       2.135802     1.508695     1.030728      21.78
 C       0.224223     0.771708     0.339022      16.26
 O      -0.550510     1.381813     1.345228     229.80
 C      -0.144169     1.939208     2.559404     119.54
 H      -0.997205     2.687126     2.982093      23.97
 H       0.104236     1.193289     3.251423      28.26
 H       0.763551     2.301595     2.502064      28.80
 C      -0.454530    -0.166351    -0.472622      12.71
 O      -1.822012    -0.283267    -0.340096     111.59
 C       0.266949    -0.757428    -1.577379      65.92
 H      -0.109801    -1.562943    -2.552375      20.41
 C       2.347551     0.212252    -0.826282      26.68
 C       3.817799     0.597573    -0.978371      90.84
 H       3.981669     0.151016    -2.005851      26.14
 O       4.255756     1.975281    -0.913943     191.59
 H       4.497478     2.088562     0.020094      26.58
 C       4.854105    -0.425951    -0.149390      77.85
 H       4.709072    -0.212756     1.065225      23.73
 O       4.387469    -1.731460    -0.362294     320.44
 H       4.371291    -1.863464    -1.347131      27.72
 C       6.376005    -0.246387    -0.449915     111.16
 O       6.872709     1.166444    -0.148485     230.72
 H       6.935472     1.264587     0.849823      29.05
 H       6.738840    -0.581348    -1.411832      32.55
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 H       6.886793    -0.959631     0.158506      31.59
55
name= lig-ACN-Water-frame_393
 C      -3.665222     0.854351    -3.463880      63.83
 H      -3.682369    -0.049410    -3.935015      28.83
 C      -3.667612     2.148529    -1.436471      72.30
 H      -3.894760     2.333855    -0.395417      27.89
 C      -3.224308     3.268690    -2.092492      18.53
 O      -3.135094     4.587565    -1.470097     180.26
 C      -3.646767     4.861469    -0.160413     124.85
 H      -3.001012     4.644785     0.586296      27.21
 H      -4.708275     4.346069    -0.046421      25.45
 H      -4.185656     5.958864    -0.175298      24.77
 C      -2.882286     3.168604    -3.512960       2.97
 O      -2.689929     4.241504    -4.262862     161.67
 H      -2.381377     5.115561    -3.867216      20.68
 C      -3.084183     1.868154    -4.216962      28.23
 H      -3.183896     1.697297    -5.275224      19.72
 C      -3.818301     0.894738    -2.133183      20.75
 C      -4.123442    -0.427105    -1.249135      58.83
 H      -4.860724    -1.124781    -1.858804      23.02
 O      -4.905286    -0.117165    -0.058973     184.19
 H      -4.154531     0.279198     0.404173      30.86
 C      -2.642472    -1.161614    -1.102829      82.51
 H      -2.319438    -1.420228    -2.181641      26.61
 C      -2.467424    -2.565858    -0.376299     112.34
 O      -3.393987    -3.481046    -1.235617     198.68
 H      -2.747858    -4.041467    -1.720025      28.77
 H      -2.968378    -2.429666     0.520299      28.20
 H      -1.430228    -2.807840    -0.411302      26.90
 C       1.653391    -0.511121    -1.706265      50.44
 H       2.056161    -1.095450    -2.526574      25.09
 C       1.599389     0.952175     0.229766      79.40
 H       2.189942     1.730028     0.824410      23.84
 C       0.241627     0.760751     0.422330      18.79
 O      -0.599383     1.383145     1.331536     199.24
 C       0.006586     1.941291     2.605231     110.60
 H      -0.941541     2.739418     2.877049      24.52
 H      -0.046279     1.180327     3.304392      28.51
 H       0.708583     2.586346     2.456136      29.54
 C      -0.469831    -0.075198    -0.549065      12.99
 O      -1.830563    -0.245803    -0.331710     144.78
 C       0.287921    -0.765729    -1.472862      60.08
 H      -0.432132    -1.737244    -2.047688      21.54
 C       2.365190     0.330306    -0.743632      23.93
 C       3.880610     0.514732    -1.037157     101.39
 H       4.081027     0.419802    -2.092692      27.61
 O       4.205691     1.921115    -0.953632     173.48
 H       4.209230     2.356110     0.017234      25.04
 C       4.805899    -0.348334    -0.148607      82.26
 H       4.666843    -0.145983     1.079767      25.59
 O       4.375628    -1.707944    -0.375893     283.06
 H       4.651265    -1.985932    -1.270484      30.87
 C       6.376854    -0.180415    -0.406120     107.79
 O       6.769155     1.128039    -0.160193     208.48
 H       7.153267     1.137833     0.766232      28.69
 H       6.535173    -0.289129    -1.530412      31.10
 H       6.882281    -0.833389     0.248099      31.36
55
name= lig-ACN-Water-frame_394
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 C      -3.687483     0.799090    -3.591149      31.53
 H      -4.114821    -0.033235    -4.115154      16.73
 C      -3.643814     2.099796    -1.412278      67.20
 H      -4.206771     2.098650    -0.415291      19.09
 C      -3.227716     3.283129    -2.095683      -5.45
 O      -3.090477     4.527698    -1.495356     163.80
 C      -3.668860     4.819917    -0.183307     123.62
 H      -2.962089     4.794749     0.611843      26.03
 H      -4.491154     4.070402     0.111510      23.90
 H      -3.786994     6.077365    -0.268164      24.29
 C      -2.849133     3.106991    -3.485164      -6.54
 O      -2.721383     4.280983    -4.379494     130.35
 H      -2.364901     5.018516    -3.901442      22.42
 C      -3.121005     1.944730    -4.172336      50.47
 H      -2.997812     2.111992    -5.297003      25.07
 C      -3.909776     0.908419    -2.069361     -21.04
 C      -4.090199    -0.332840    -1.277774      88.50
 H      -4.706024    -1.216741    -1.883436      24.68
 O      -4.851588    -0.048972    -0.064099     148.88
 H      -4.525291     0.203671     0.783684      23.41
 C      -2.603822    -1.097415    -1.025692      89.33
 H      -2.142835    -1.084057    -2.118171      28.56
 C      -2.526487    -2.503396    -0.381946     127.13
 O      -3.343004    -3.422539    -1.163544     256.83
 H      -2.924139    -3.845670    -1.870635      31.61
 H      -2.822242    -2.637434     0.658250      27.57
 H      -1.551516    -2.985354    -0.310419      27.25
 C       1.668139    -0.561590    -1.598121      33.69
 H       2.285315    -0.928994    -2.427096      19.70
 C       1.623327     1.049497     0.228096      53.61
 H       2.041256     1.837927     1.047244      22.05
 C       0.205774     0.745020     0.430655      -4.19
 O      -0.610813     1.410747     1.370488     194.34
 C       0.029526     1.967292     2.581814     111.26
 H      -0.828087     2.748368     3.160561      23.45
 H       0.410961     1.274309     3.282706      28.04
 H       0.918592     2.371693     2.405757      27.57
 C      -0.468380    -0.019877    -0.535908      10.48
 O      -1.844865    -0.149249    -0.296047     153.92
 C       0.292278    -0.781681    -1.413411      67.85
 H      -0.239272    -1.692978    -2.228470      20.93
 C       2.362469     0.363898    -0.853695      16.61
 C       3.894545     0.527339    -1.071131     116.80
 H       4.105702     0.152838    -1.976663      27.36
 O       4.163571     1.960956    -0.973204     208.74
 H       4.092722     2.148750     0.055856      22.75
 C       4.793198    -0.303439    -0.156835      81.63
 H       4.413273     0.071504     0.978139      23.32
 O       4.404468    -1.745925    -0.362571     299.37
 H       4.583562    -1.831272    -1.377696      26.16
 C       6.253083    -0.184931    -0.404071     108.34
 O       6.748432     1.194447    -0.121279     280.20
 H       6.875998     1.296239     0.875371      29.71
 H       6.430315    -0.456261    -1.541399      30.53
 H       6.823505    -0.978962    -0.000068      31.25
55
name= lig-ACN-Water-frame_395
 C      -3.698379     0.800484    -3.530040      79.45
 H      -4.095672    -0.023499    -4.213098      17.91
 C      -3.710181     2.099417    -1.419715      41.41
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 H      -3.635365     2.153690    -0.237421      24.90
 C      -3.193769     3.224989    -2.104365      12.35
 O      -3.031655     4.501992    -1.556416     176.40
 C      -3.632857     4.767385    -0.207862     105.71
 H      -2.773131     4.406678     0.428651      23.71
 H      -4.576402     4.241163     0.041381      24.75
 H      -4.083205     5.959819    -0.138150      23.52
 C      -2.935051     3.261390    -3.494491       2.41
 O      -2.695454     4.232586    -4.412251     142.42
 H      -2.774076     5.157409    -4.043434      18.44
 C      -3.202225     1.990580    -4.184201     -28.72
 H      -2.849625     1.960421    -5.313589      27.31
 C      -3.903650     0.869794    -2.183137      12.43
 C      -4.006964    -0.364430    -1.218813      56.44
 H      -4.699345    -1.197604    -1.852202      23.88
 O      -4.814587     0.002446    -0.063896     175.63
 H      -4.034726     0.221185     0.495852      27.57
 C      -2.662038    -0.971685    -1.019915      69.54
 H      -2.216163    -1.098666    -2.129042      28.13
 C      -2.605198    -2.468940    -0.391785     122.79
 O      -3.357010    -3.417911    -1.110567     215.37
 H      -2.757266    -3.563914    -1.940860      28.17
 H      -3.075396    -2.284269     0.617773      27.62
 H      -1.532489    -2.551768    -0.457159      27.23
 C       1.683764    -0.602325    -1.550746      51.83
 H       2.112773    -1.355525    -2.244322      19.94
 C       1.608978     1.063605     0.210447      69.07
 H       2.321027     1.750582     0.913389      20.51
 C       0.261414     0.875389     0.411105       2.82
 O      -0.582667     1.430322     1.437417     193.73
 C       0.113034     1.965686     2.548159     105.93
 H      -0.710255     2.768332     3.198180      24.16
 H       0.279382     1.106194     3.170167      27.06
 H       0.775666     2.699682     2.227003      26.45
 C      -0.470650    -0.079448    -0.439097     -34.41
 O      -1.815314    -0.018556    -0.222223     116.43
 C       0.287763    -0.804784    -1.444329      48.93
 H      -0.218651    -1.552819    -2.381377      23.46
 C       2.330951     0.411050    -0.809206      34.02
 C       3.789266     0.617670    -1.109708     107.03
 H       4.004486     0.485130    -2.047531      29.38
 O       4.146942     2.002608    -0.989321     192.40
 H       4.372575     2.305848    -0.103824      29.02
 C       4.676960    -0.370479    -0.128179      59.32
 H       4.601340    -0.267522     1.121539      22.29
 O       4.453366    -1.727381    -0.329207     290.63
 H       4.458321    -2.009112    -1.349996      27.23
 C       6.217605    -0.127497    -0.433085      93.70
 O       6.742668     1.220867    -0.075202     230.55
 H       6.869360     1.223024     0.903289      29.70
 H       6.453575    -0.124323    -1.613523      28.11
 H       6.719907    -0.814943     0.214590      29.79
55
name= lig-ACN-Water-frame_396
 C      -3.689738     0.906012    -3.544846      59.46
 H      -3.515643    -0.157463    -4.016395      26.77
 C      -3.667208     2.103672    -1.529049      69.39
 H      -3.585427     2.113811    -0.353975      24.93
 C      -3.210474     3.274889    -2.163471      13.93
 O      -3.026309     4.539577    -1.555028     191.85
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 C      -3.556560     4.653605    -0.266211     115.83
 H      -3.061701     4.424193     0.771412      24.55
 H      -4.476871     4.089548    -0.287033      26.27
 H      -3.600989     5.906815    -0.142082      24.45
 C      -3.127867     3.187223    -3.616922      19.76
 O      -2.642914     4.273794    -4.398482     111.50
 H      -2.691002     5.224412    -3.935364      22.79
 C      -3.240487     1.986527    -4.204740      55.42
 H      -3.288914     1.825504    -5.377313      14.23
 C      -3.868363     0.882136    -2.091824       6.37
 C      -4.093572    -0.333550    -1.285053     101.72
 H      -4.705839    -1.336791    -1.712628      22.76
 O      -4.708544    -0.003896    -0.048839     153.82
 H      -4.414126     0.632452     0.701869      22.31
 C      -2.652162    -0.915019    -1.013095      91.84
 H      -2.164760    -0.985291    -2.111029      29.69
 C      -2.623821    -2.238483    -0.351955     108.90
 O      -3.377296    -3.435078    -1.111182     124.50
 H      -2.903860    -3.872674    -1.938585      25.47
 H      -3.153962    -2.422379     0.686523      26.50
 H      -1.718194    -2.771728    -0.071426      27.79
 C       1.620799    -0.667692    -1.545198      58.94
 H       2.352303    -1.171183    -2.210725      19.74
 C       1.638096     1.102606     0.211840      70.69
 H       2.165043     1.904335     0.838345      20.65
 C       0.226289     0.913605     0.410708      14.20
 O      -0.541163     1.432450     1.394033     194.77
 C       0.171097     2.012029     2.580548      90.09
 H      -0.849631     2.510818     3.175003      23.00
 H       0.789217     1.359476     3.262086      25.93
 H       1.108679     2.639499     2.298750      22.68
 C      -0.371042    -0.070355    -0.388619      -2.59
 O      -1.859686    -0.007010    -0.204936      89.50
 C       0.229873    -0.762595    -1.393381      61.09
 H      -0.460524    -1.581709    -1.951851      25.61
 C       2.264017     0.363582    -0.791252      26.28
 C       3.748037     0.626395    -1.033277      99.24
 H       3.894873     0.302526    -1.916924      30.31
 O       4.178886     2.060167    -0.995853     190.77
 H       4.339435     2.246108    -0.085178      28.96
 C       4.696607    -0.298655    -0.204781      71.98
 H       4.315532     0.050751     0.933976      24.92
 O       4.445011    -1.783672    -0.323844     313.20
 H       4.809416    -1.921687    -1.311343      26.45
 C       6.220022    -0.005970    -0.402466     101.54
 O       6.727282     1.246053    -0.011918     271.58
 H       7.017990     1.200196     0.938233      27.77
 H       6.386084    -0.260940    -1.598788      30.01
 H       6.806837    -0.869270    -0.056788      31.48
55
name= lig-ACN-Water-frame_397
 C      -3.632719     0.768365    -3.487087      11.95
 H      -3.691893    -0.264561    -4.046839      16.50
 C      -3.562519     2.208844    -1.498483      37.16
 H      -3.907877     2.351242    -0.440394      21.93
 C      -3.299871     3.347309    -2.299851      16.71
 O      -2.950341     4.505104    -1.613950     208.86
 C      -3.579474     4.613791    -0.238614     101.05
 H      -2.824733     3.837046     0.276572      22.89
 H      -4.608139     4.383957    -0.160943      27.65
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 H      -3.620452     5.808946     0.011703      24.48
 C      -3.165524     3.308051    -3.688784      -5.66
 O      -2.622278     4.327349    -4.371022     100.01
 H      -2.429175     5.090766    -3.720279      21.72
 C      -3.324590     1.961275    -4.351846     -37.87
 H      -3.057672     2.048540    -5.494359      21.54
 C      -3.871812     0.965264    -2.163193      44.64
 C      -4.049880    -0.255268    -1.240266      84.75
 H      -4.809851    -0.955032    -1.906380      23.21
 O      -4.734295    -0.066513     0.012562     133.85
 H      -4.090315     0.595159     0.394432      27.39
 C      -2.593243    -0.926018    -1.064178      73.11
 H      -2.082342    -1.002309    -2.122977      27.63
 C      -2.722127    -2.350371    -0.298283     112.50
 O      -3.381238    -3.356955    -1.087260     242.50
 H      -2.662689    -3.734139    -1.550900      31.05
 H      -3.437082    -1.876814     0.527944      25.53
 H      -1.613874    -2.430100    -0.031028      25.85
 C       1.591899    -0.627198    -1.528922      42.15
 H       1.947408    -1.216485    -2.394253      22.37
 C       1.578830     1.149588     0.219724      71.08
 H       2.070907     1.932194     0.712441      22.69
 C       0.278114     0.859683     0.442352      20.61
 O      -0.490182     1.494599     1.449631     202.47
 C       0.208141     2.024290     2.588937      93.16
 H      -0.529954     2.671758     3.384300      23.95
 H       0.575620     1.059991     3.089611      25.02
 H       0.842156     2.986345     2.118211      22.40
 C      -0.550467     0.027842    -0.377476      13.00
 O      -1.841535    -0.038086    -0.207739     151.84
 C       0.208430    -0.834550    -1.335637      54.40
 H      -0.237723    -1.689477    -1.900347      23.71
 C       2.293156     0.329015    -0.768756      20.08
 C       3.782552     0.564271    -1.095830     115.33
 H       3.953339     0.432147    -2.026144      26.46
 O       4.196521     2.001668    -0.983856     239.55
 H       4.161273     2.378043    -0.052163      23.61
 C       4.730639    -0.218503    -0.163855      75.06
 H       4.579015    -0.111203     1.055138      21.26
 O       4.461300    -1.716945    -0.339945     277.49
 H       4.640477    -2.058050    -1.289622      27.67
 C       6.212418    -0.017562    -0.441222      84.38
 O       6.749044     1.313932     0.060261     253.35
 H       6.782391     1.335006     1.079526      28.29
 H       6.436330     0.239476    -1.597966      26.57
 H       6.754182    -0.840741     0.097217      28.25
55
name= lig-ACN-Water-frame_398
 C      -3.570663     0.841912    -3.613179      11.46
 H      -3.968776    -0.110323    -4.040914      17.65
 C      -3.634052     2.268976    -1.559012      72.44
 H      -3.701720     2.338381    -0.524678      23.22
 C      -3.354112     3.384887    -2.331067       6.19
 O      -2.954795     4.551901    -1.672741     176.26
 C      -3.521545     4.597292    -0.278212     111.23
 H      -3.091891     3.821879     0.619501      22.88
 H      -4.571302     4.414019    -0.316072      27.12
 H      -3.089457     5.523622     0.211182      25.66
 C      -3.117502     3.229273    -3.746995      19.82
 O      -2.598886     4.421908    -4.395367     145.05
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 H      -2.604427     5.200545    -3.833958      21.65
 C      -3.329530     1.975769    -4.340089      73.41
 H      -3.017916     1.642692    -5.359005      27.44
 C      -3.805257     1.035420    -2.136957      17.65
 C      -3.967694    -0.225665    -1.279196      92.27
 H      -4.629515    -1.062895    -1.846741      24.54
 O      -4.717623    -0.079628     0.029560     161.43
 H      -4.316009     0.109864     0.872565      23.85
 C      -2.688848    -1.000592    -1.093765      93.45
 H      -2.166366    -1.169154    -2.088849      27.72
 C      -2.807096    -2.261593    -0.260919     115.51
 O      -3.343008    -3.301142    -1.072357     216.13
 H      -2.741810    -3.876934    -1.588710      27.23
 H      -3.504041    -2.360488     0.716968      23.78
 H      -1.942412    -2.862376     0.250204      24.18
 C       1.532784    -0.576178    -1.509783      54.57
 H       2.146728    -1.184766    -2.180389      20.51
 C       1.636270     1.081542     0.153024      61.63
 H       2.093749     1.730090     0.752246      20.84
 C       0.175407     0.857202     0.510782      -2.20
 O      -0.545987     1.554303     1.488276     204.97
 C       0.227254     2.031598     2.587785      93.51
 H      -0.674789     2.437518     3.280868      22.98
 H       0.967496     1.341101     3.240501      24.05
 H       1.233229     2.754334     2.281400      20.49
 C      -0.493979    -0.008430    -0.444624      14.20
 O      -1.930663    -0.070550    -0.187240     129.58
 C       0.177636    -0.845726    -1.235593      82.47
 H      -0.275836    -1.504870    -1.850203      25.41
 C       2.339395     0.364253    -0.792288      25.38
 C       3.834779     0.593578    -1.088771     100.92
 H       4.009339     0.219565    -1.972698      27.89
 O       4.163214     1.935932    -0.994051     243.18
 H       4.359733     2.152083     0.029960      21.35
 C       4.773406    -0.308910    -0.171192      81.28
 H       4.526427     0.072472     0.970834      22.00
 O       4.477561    -1.608624    -0.319779     341.17
 H       4.560222    -1.738236    -1.271665      27.39
 C       6.287006     0.114815    -0.432716      86.23
 O       6.758444     1.348677     0.104629     293.00
 H       6.826846     1.291314     1.132461      28.97
 H       6.470815    -0.087195    -1.619658      29.23
 H       6.938496    -0.793322    -0.126467      28.71
55
name= lig-ACN-Water-frame_399
 C      -3.672914     0.940883    -3.539295      60.44
 H      -3.666937     0.039582    -4.090221      27.25
 C      -3.754847     2.238647    -1.601833      70.72
 H      -3.606880     2.204591    -0.599565      27.85
 C      -3.301141     3.406771    -2.350455       6.40
 O      -3.018792     4.607375    -1.680491     206.92
 C      -3.410637     4.641122    -0.329372     118.76
 H      -3.072828     3.602364     0.283686      23.48
 H      -4.484358     4.829395    -0.273737      26.86
 H      -3.120985     5.579009    -0.005713      28.04
 C      -3.013285     3.324817    -3.751349       7.03
 O      -2.610284     4.415178    -4.452916     165.66
 H      -2.889285     5.212670    -3.970561      24.51
 C      -3.186817     2.047374    -4.401007      33.35
 H      -3.285960     2.119482    -5.453845      19.42
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 C      -3.726261     0.947524    -2.174832       2.19
 C      -4.022465    -0.274752    -1.281306      79.49
 H      -4.760550    -0.922841    -1.897577      23.66
 O      -4.720775    -0.069557    -0.036813     150.93
 H      -3.981875     0.201448     0.562679      25.11
 C      -2.709061    -1.002296    -0.943141      86.72
 H      -2.276867    -1.277623    -1.906679      29.30
 C      -2.858302    -2.314845    -0.171133     107.56
 O      -3.400537    -3.367649    -1.135219     150.45
 H      -2.554268    -3.668028    -1.715809      25.91
 H      -3.705735    -1.986626     0.544424      25.99
 H      -1.728217    -2.254898     0.240451      25.01
 C       1.619482    -0.626309    -1.528665      42.41
 H       2.051646    -1.306319    -2.261146      19.17
 C       1.552385     1.041374     0.282125      68.15
 H       2.135185     1.655163     0.866005      21.73
 C       0.212597     0.902549     0.434905      20.91
 O      -0.568867     1.535125     1.453705     182.28
 C       0.278154     2.043759     2.656104      82.62
 H      -0.369336     2.672578     3.353305      25.85
 H       0.539844     0.975145     3.110179      23.41
 H       0.932824     2.867976     2.159369      22.53
 C      -0.583080    -0.015318    -0.269197       1.69
 O      -1.923098    -0.095754    -0.214112     146.54
 C       0.213721    -0.844814    -1.289213      52.71
 H      -0.238831    -1.533645    -1.755847      28.23
 C       2.279514     0.373406    -0.839161      28.06
 C       3.833839     0.513234    -1.054879     110.72
 H       4.009400     0.322524    -2.007536      29.96
 O       4.152615     1.973990    -1.025708     199.17
 H       4.574430     2.288910    -0.124442      24.10
 C       4.841010    -0.149041    -0.156115      66.74
 H       4.582131     0.028528     0.995607      23.87
 O       4.495383    -1.640731    -0.314453     338.43
 H       4.802615    -2.028215    -1.126509      32.66
 C       6.359749     0.104963    -0.428382      93.92
 O       6.764311     1.400247     0.105481     251.89
 H       7.227493     1.281252     0.986503      29.32
 H       6.486169     0.404428    -1.555833      29.81
 H       7.035248    -0.711771     0.049735      29.29
55
name= lig-ACN-Water-frame_400
 C      -3.620018     0.946465    -3.680287      58.74
 H      -3.710981     0.036310    -4.141795      36.01
 C      -3.710261     2.258441    -1.596231      77.59
 H      -4.221146     2.499960    -0.696830      27.10
 C      -3.233325     3.347849    -2.304342      15.14
 O      -3.074069     4.633409    -1.761943     187.81
 C      -3.398028     4.779626    -0.332329     128.16
 H      -2.820297     3.800810     0.241740      25.61
 H      -4.440542     4.610457    -0.042060      27.36
 H      -2.840012     5.416593     0.105512      29.93
 C      -2.961550     3.379032    -3.684623      22.73
 O      -2.629634     4.445271    -4.539028     110.22
 H      -2.578292     5.387519    -4.071223      20.95
 C      -3.157232     2.145072    -4.342182      43.58
 H      -3.103506     2.041723    -5.380013      18.09
 C      -3.799914     0.959062    -2.200004     -29.05
 C      -4.076922    -0.344197    -1.336800      87.74
 H      -4.660169    -1.090686    -1.888903      25.29
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 O      -4.731426     0.002598    -0.107739     151.93
 H      -4.321147     0.716738     0.516315      24.69
 C      -2.718803    -1.051995    -0.973292      76.60
 H      -2.144671    -1.210569    -1.834707      28.96
 C      -2.951594    -2.376138    -0.173166     114.17
 O      -3.366611    -3.386074    -1.108011     202.82
 H      -2.705015    -3.602054    -1.778471      28.26
 H      -3.662832    -2.475713     0.670346      25.63
 H      -2.074482    -3.029242     0.368792      24.56
 C       1.578897    -0.682956    -1.533631      52.21
 H       2.101264    -1.206822    -2.338152      19.25
 C       1.617581     1.002082     0.293746      58.95
 H       2.148825     1.753487     0.930776      20.89
 C       0.130500     0.924847     0.476491      -4.32
 O      -0.553074     1.560533     1.469637     205.12
 C       0.199289     2.020263     2.572851     109.48
 H      -0.520541     2.570785     3.124490      26.60
 H       0.726900     1.201430     3.313744      25.19
 H       1.175786     2.517422     2.360173      24.26
 C      -0.463482    -0.146380    -0.350809       1.16
 O      -1.923318    -0.043512    -0.145255      82.86
 C       0.199277    -0.810015    -1.296376      82.85
 H      -0.175848    -1.539432    -1.719138      29.30
 C       2.285533     0.323448    -0.732596      16.06
 C       3.785527     0.628244    -1.059372      87.90
 H       3.963615     0.157848    -1.971680      25.86
 O       4.148297     2.052582    -1.105556     231.85
 H       4.291590     2.327233    -0.183652      26.65
 C       4.858536    -0.223877    -0.125914      74.21
 H       4.800738     0.122847     0.978607      23.66
 O       4.571766    -1.641992    -0.236408     334.58
 H       4.744264    -1.771665    -1.189565      27.98
 C       6.364066     0.159265    -0.459261      88.49
 O       6.819205     1.481609     0.101870     254.78
 H       7.043377     1.325438     1.070666      28.79
 H       6.585441    -0.006311    -1.575056      31.93
 H       6.920566    -0.787086    -0.041281      30.37
55
name= lig-ACN-Water-frame_401
 C      -3.483763     0.929905    -3.660143      46.50
 H      -3.724190     0.193818    -4.337819      16.70
 C      -3.693952     2.224960    -1.590225      21.91
 H      -4.357203     2.318378    -0.689889      19.62
 C      -3.174018     3.446742    -2.277022       2.20
 O      -3.162496     4.706556    -1.750082     184.40
 C      -3.318654     4.754688    -0.308789     115.98
 H      -2.777261     3.870772     0.324011      24.97
 H      -4.436277     4.877624    -0.148347      25.87
 H      -3.220601     5.766479     0.002718      27.91
 C      -2.931617     3.353181    -3.736189       6.93
 O      -2.636416     4.480773    -4.555113     140.89
 H      -2.594117     5.340818    -3.943640      17.73
 C      -3.173829     2.136058    -4.329164      51.69
 H      -2.730282     2.088518    -5.300276      27.89
 C      -3.903001     0.976837    -2.331118      35.57
 C      -4.018397    -0.269801    -1.390847      73.97
 H      -4.647007    -1.010422    -1.756726      29.48
 O      -4.826095     0.071336    -0.166744      90.63
 H      -4.421263     0.823861     0.272337      28.00
 C      -2.686123    -1.054112    -0.930927      77.37
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 H      -2.257402    -1.339159    -1.826119      31.77
 C      -2.974602    -2.494819    -0.171551     107.80
 O      -3.397268    -3.453495    -1.144315     214.36
 H      -2.691285    -3.715886    -1.719772      29.81
 H      -3.794711    -2.229461     0.407591      28.62
 H      -1.892170    -2.561008     0.442810      26.28
 C       1.611473    -0.596456    -1.472111      45.30
 H       2.148640    -1.158015    -2.257793      26.51
 C       1.575224     0.991829     0.282480      64.13
 H       2.171423     1.792423     0.902608      22.04
 C       0.270818     0.788501     0.490797      36.65
 O      -0.547885     1.551667     1.413037     207.07
 C       0.173202     2.046733     2.593161     120.49
 H      -0.507512     2.659221     3.053013      28.97
 H       0.256706     1.104729     3.284850      26.67
 H       0.921653     2.728753     2.304502      27.50
 C      -0.541657    -0.024352    -0.309188       3.36
 O      -1.899977    -0.099997    -0.124812      93.97
 C       0.195301    -0.931151    -1.362727      47.52
 H      -0.265529    -1.526032    -1.984630      25.39
 C       2.335279     0.253062    -0.660089      32.01
 C       3.797165     0.639288    -1.015904      97.59
 H       3.946035     0.463343    -2.085146      23.94
 O       4.093864     2.091013    -1.161452     246.58
 H       4.266925     2.492306    -0.332765      27.61
 C       4.843320    -0.176352    -0.122996      87.64
 H       4.551893     0.023091     0.946663      23.22
 O       4.675212    -1.589053    -0.153559     318.12
 H       4.673652    -2.069117    -1.030086      28.26
 C       6.354264     0.172538    -0.445416      95.69
 O       6.850809     1.476090     0.030954     259.27
 H       6.932268     1.455809     1.047137      28.10
 H       6.514588     0.301293    -1.518788      28.81
 H       7.101289    -0.525728     0.093793      27.05
55
name= lig-ACN-Water-frame_402
 C      -3.465046     0.912646    -3.689009      47.71
 H      -3.341055    -0.103533    -4.045702      29.56
 C      -3.713740     2.298452    -1.733524      77.76
 H      -3.629310     2.386050    -0.575183      27.86
 C      -3.254357     3.422945    -2.332062      22.39
 O      -3.189843     4.758943    -1.682819     200.62
 C      -3.419029     4.778095    -0.281196     129.75
 H      -2.588628     4.090718     0.274371      25.83
 H      -4.334495     4.194251     0.061140      25.56
 H      -3.062358     5.809485     0.172484      25.55
 C      -2.945519     3.418542    -3.697247       2.76
 O      -2.633449     4.465140    -4.479560     102.19
 H      -2.896411     5.354186    -4.051089      22.12
 C      -3.037898     2.097229    -4.420209       4.30
 H      -3.039689     2.043338    -5.554697      15.50
 C      -3.808544     1.009667    -2.287380       5.49
 C      -4.051150    -0.228334    -1.377072      90.10
 H      -4.484545    -0.878120    -1.998178      28.02
 O      -4.895086     0.142323    -0.271088     171.75
 H      -4.353210     0.623262     0.384218      28.47
 C      -2.723514    -1.028286    -0.948033     102.85
 H      -2.157285    -1.176685    -1.809261      30.51
 C      -2.994577    -2.358923    -0.222632     103.08
 O      -3.405087    -3.535496    -1.181259     148.21
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 H      -2.562729    -3.965924    -1.651116      25.89
 H      -3.723599    -2.414720     0.472215      28.57
 H      -2.063044    -2.860308     0.448937      24.93
 C       1.605220    -0.647398    -1.471020      52.74
 H       2.136675    -1.204864    -2.271992      24.23
 C       1.666003     1.004688     0.333125      44.17
 H       2.164774     1.849149     1.007253      21.41
 C       0.208906     0.714526     0.534541      -7.01
 O      -0.513758     1.531971     1.329431     184.97
 C       0.063661     2.111584     2.620641     119.77
 H      -0.623930     2.708250     3.051889      28.87
 H       0.469598     1.311513     3.316673      27.55
 H       0.942575     2.564798     2.461384      28.34
 C      -0.518736    -0.138572    -0.442156      17.80
 O      -1.898226    -0.200530    -0.112465     167.60
 C       0.216981    -0.819701    -1.276059      86.70
 H      -0.179394    -1.447638    -1.998319      26.63
 C       2.375847     0.293897    -0.664795      17.65
 C       3.828798     0.578513    -1.043866      89.65
 H       3.977045     0.026856    -2.058222      24.98
 O       4.009193     2.095448    -1.134549     170.08
 H       4.462846     2.352150    -0.259957      24.42
 C       4.878443    -0.047370    -0.093274     113.04
 H       4.731114     0.343957     0.902718      27.82
 O       4.730557    -1.577214    -0.068218     240.33
 H       5.067947    -1.734190    -1.020972      27.71
 C       6.355549     0.223100    -0.405146     102.63
 O       6.848497     1.508018    -0.046089     239.79
 H       7.148868     1.499679     0.929024      28.16
 H       6.399606     0.184013    -1.482059      33.56
 H       6.850299    -0.749991    -0.119338      32.63
55
name= lig-ACN-Water-frame_403
 C      -3.403544     0.941593    -3.674116      73.16
 H      -3.352585    -0.052725    -4.239306      26.11
 C      -3.675488     2.333557    -1.677757      46.12
 H      -3.611622     2.291171    -0.491846      28.11
 C      -3.370833     3.555623    -2.377573      11.65
 O      -3.220395     4.713157    -1.690769     151.25
 C      -3.435326     4.677032    -0.173517      98.37
 H      -2.461948     4.306474     0.256473      25.90
 H      -4.419148     4.215295     0.214215      24.35
 H      -3.843526     5.880935    -0.060595      24.17
 C      -2.997599     3.323185    -3.806180       5.52
 O      -2.618919     4.505650    -4.442784      93.89
 H      -2.765887     5.349288    -3.907837      22.79
 C      -2.991593     2.063715    -4.385063      64.26
 H      -2.887466     2.129343    -5.563424      18.53
 C      -3.609340     1.055200    -2.290667      17.78
 C      -4.041396    -0.201563    -1.438956      80.12
 H      -4.642346    -0.832766    -1.876098      28.88
 O      -4.933994     0.210372    -0.357323     138.61
 H      -4.453195     0.180095     0.557963      25.93
 C      -2.793021    -1.006895    -1.041559      76.30
 H      -2.385620    -1.274202    -2.000961      28.71
 C      -3.054334    -2.411934    -0.325704     108.22
 O      -3.379666    -3.517334    -1.165938     199.69
 H      -2.586912    -3.890187    -1.654024      27.72
 H      -3.775703    -2.234632     0.369048      28.45
 H      -1.919774    -2.597319     0.144774      25.27
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 C       1.699154    -0.657743    -1.441348      47.84
 H       2.171727    -1.246175    -2.253176      20.56
 C       1.624756     0.910243     0.362238      73.56
 H       2.145698     1.687630     1.027095      22.79
 C       0.285590     0.765978     0.484947      22.90
 O      -0.534822     1.563063     1.386173     203.94
 C       0.017654     2.122731     2.563460     141.10
 H      -0.845302     2.635613     2.827270      29.05
 H       0.073237     1.351710     3.315662      28.05
 H       0.714969     2.796116     2.437605      29.69
 C      -0.492660    -0.133689    -0.267531      -5.08
 O      -1.884350    -0.265593    -0.090414     111.20
 C       0.285197    -0.828919    -1.388732      41.82
 H      -0.241819    -1.672808    -1.927942      25.66
 C       2.347619     0.296651    -0.714214      39.73
 C       3.826874     0.554841    -1.046047      82.78
 H       4.176980     0.228666    -2.161482      26.56
 O       3.975747     1.985426    -1.099817     145.03
 H       4.273739     2.328331    -0.125847      24.93
 C       4.891625    -0.034204     0.006874      92.39
 H       4.698527     0.281493     0.975031      28.54
 O       4.782878    -1.437231     0.016871     315.60
 H       4.829059    -1.932066    -0.869042      29.19
 C       6.344803     0.218694    -0.497604     106.56
 O       6.884124     1.577248    -0.086209     188.60
 H       7.185652     1.458987     0.852028      28.47
 H       6.485212     0.087959    -1.536228      33.24
 H       7.026720    -0.366411     0.102995      31.02
55
name= lig-ACN-Water-frame_404
 C      -3.270603     0.934301    -3.647194      34.27
 H      -3.719052    -0.006560    -4.218481      20.03
 C      -3.540946     2.305796    -1.601978      55.92
 H      -4.171925     2.362486    -0.647133      19.69
 C      -3.453321     3.421373    -2.373263      19.62
 O      -3.282454     4.698110    -1.665823     183.69
 C      -3.490222     4.654511    -0.202305     111.80
 H      -2.681542     4.551311     0.502086      26.26
 H      -4.156025     3.771143    -0.045014      23.05
 H      -3.886294     5.870886     0.094788      24.28
 C      -3.061182     3.458140    -3.758047       8.55
 O      -2.577401     4.479808    -4.496791     168.50
 H      -2.793181     5.327873    -4.047099      20.02
 C      -3.012197     2.132345    -4.414160      35.48
 H      -2.411272     1.868882    -5.415190      25.59
 C      -3.553785     1.068002    -2.280000      28.13
 C      -4.007001    -0.113328    -1.505888      87.98
 H      -4.431883    -0.632385    -2.216474      31.97
 O      -4.945501     0.249599    -0.382522     128.91
 H      -4.439047     0.088447     0.433710      25.21
 C      -2.794854    -1.078355    -1.123678      78.48
 H      -2.142889    -1.116984    -2.023597      29.71
 C      -3.021684    -2.378226    -0.383188     114.32
 O      -3.393758    -3.520837    -1.187441     227.47
 H      -2.770800    -3.706735    -1.843481      31.55
 H      -3.829935    -2.415168     0.283058      27.33
 H      -2.064912    -2.608620     0.349605      26.12
 C       1.675240    -0.702002    -1.536439      43.29
 H       2.329296    -1.220694    -2.244302      21.78
 C       1.666426     0.888446     0.360562      58.04
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 H       2.275737     1.510452     1.035357      23.55
 C       0.210305     0.830994     0.517498      -0.91
 O      -0.548343     1.541806     1.357669     211.37
 C      -0.079714     2.198907     2.589097     130.67
 H      -0.732892     2.890300     3.094594      27.75
 H       0.297910     1.494916     3.270838      29.29
 H       0.725401     2.705046     2.400997      30.07
 C      -0.445702    -0.223291    -0.330332      -9.26
 O      -1.857532    -0.299966    -0.106372      73.02
 C       0.250919    -0.860744    -1.300798      69.97
 H      -0.232555    -1.708935    -1.998467      25.05
 C       2.388425     0.219816    -0.709508      15.35
 C       3.833735     0.566285    -0.925802      88.62
 H       3.963383     0.064716    -2.066417      24.27
 O       4.008115     1.974730    -1.051629     179.56
 H       3.955247     2.366428    -0.119601      28.08
 C       4.905071    -0.012362    -0.032626     107.22
 H       4.797069     0.421254     0.873929      30.45
 O       4.778436    -1.429860     0.136305     308.90
 H       4.780968    -1.726939    -0.794659      30.20
 C       6.426563     0.308598    -0.456985      98.30
 O       6.904877     1.640793    -0.154990     249.50
 H       7.104337     1.603973     0.807272      29.75
 H       6.423792     0.247658    -1.517782      32.47
 H       6.940792    -0.533242    -0.064481      32.52
55
name= lig-ACN-Water-frame_405
 C      -3.224810     1.034662    -3.650520      75.90
 H      -3.124364    -0.073446    -4.138792      26.78
 C      -3.539343     2.233179    -1.604163      78.96
 H      -3.866845     2.188984    -0.566575      26.06
 C      -3.350002     3.491549    -2.299953       6.77
 O      -3.355705     4.671692    -1.661046     184.99
 C      -3.570124     4.651633    -0.273969     122.18
 H      -2.612140     4.536844     0.057476      28.76
 H      -4.275232     3.966379     0.258278      25.42
 H      -4.247900     5.757901     0.053528      24.24
 C      -3.058840     3.416844    -3.739335      -0.45
 O      -2.551616     4.481367    -4.553537     -61.47
 H      -2.892005     5.351927    -4.291415      24.21
 C      -2.980694     2.182100    -4.352297      58.75
 H      -2.695652     2.378497    -5.475241      18.50
 C      -3.538464     1.052342    -2.268648      32.24
 C      -3.989060    -0.183845    -1.529875      84.66
 H      -4.618397    -0.764066    -2.006905      30.07
 O      -4.887515     0.221384    -0.452682     168.16
 H      -4.476602     0.242892     0.405019      29.00
 C      -2.670296    -1.019559    -1.097835      88.50
 H      -2.211804    -1.357761    -2.110558      28.08
 C      -3.025412    -2.382992    -0.355120     100.49
 O      -3.430434    -3.560389    -1.270621     173.04
 H      -2.817929    -3.722606    -2.083487      27.47
 H      -3.848218    -2.102613     0.364290      26.46
 H      -2.077632    -2.782284     0.129142      26.18
 C       1.628395    -0.686264    -1.559390      59.37
 H       1.922334    -1.249783    -2.421725      28.14
 C       1.633014     0.896349     0.369908      66.59
 H       2.130037     1.527678     1.049982      23.31
 C       0.253023     0.728667     0.477558      10.75
 O      -0.643341     1.556356     1.360775     156.70
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 C      -0.003959     2.255646     2.594004     113.33
 H      -0.963589     2.785022     2.854500      26.21
 H       0.167005     1.547753     3.285867      29.86
 H       0.739577     2.860586     2.333903      29.40
 C      -0.484058    -0.165445    -0.358158      16.69
 O      -1.846884    -0.323300    -0.169228     153.25
 C       0.308487    -0.983546    -1.262880      49.31
 H      -0.361907    -1.748815    -2.016709      21.37
 C       2.336264     0.119839    -0.623979      29.16
 C       3.828734     0.518664    -0.925660      68.74
 H       4.259186     0.176450    -2.071111      23.34
 O       4.041479     2.068435    -0.992679     181.79
 H       4.208291     2.406624    -0.119518      27.15
 C       4.998593     0.056247     0.042266      97.47
 H       4.889837     0.416964     0.963142      28.83
 O       4.751130    -1.470854     0.218060     285.78
 H       5.019342    -1.928210    -0.595959      29.90
 C       6.409974     0.359125    -0.493039     110.13
 O       6.922001     1.689780    -0.152413     209.60
 H       7.254349     1.742282     0.788868      28.18
 H       6.491335     0.254659    -1.569124      33.15
 H       7.128042    -0.290805    -0.096515      32.39
55
name= lig-ACN-Water-frame_406
 C      -3.179877     0.986640    -3.677468      61.72
 H      -2.743475     0.093113    -4.326204      25.88
 C      -3.579784     2.307057    -1.614275      62.94
 H      -3.388207     2.348889    -0.605382      32.69
 C      -3.198837     3.450644    -2.293691      10.33
 O      -3.474211     4.723949    -1.703617     175.85
 C      -3.641330     4.706815    -0.221926     114.86
 H      -2.852058     4.630498     0.414148      28.45
 H      -4.352967     3.909044    -0.051659      24.72
 H      -3.949437     5.986418    -0.095205      24.22
 C      -2.949360     3.499887    -3.685751      19.77
 O      -2.598928     4.484142    -4.552092     108.04
 H      -2.778554     5.374294    -4.105366      21.47
 C      -2.950395     2.226220    -4.349375      18.60
 H      -2.979318     2.079167    -5.453416      17.47
 C      -3.546834     0.983467    -2.349440     -14.64
 C      -3.905637    -0.325172    -1.503357      82.58
 H      -4.284383    -1.011827    -2.137540      28.85
 O      -4.836912     0.158023    -0.480719     138.66
 H      -4.295542     0.314153     0.376429      27.64
 C      -2.678108    -1.099799    -1.084793      88.76
 H      -2.012895    -1.200206    -2.068004      27.18
 C      -2.999661    -2.475834    -0.433170     113.19
 O      -3.502597    -3.510361    -1.303998     203.01
 H      -2.684311    -3.724237    -1.948710      26.26
 H      -3.894525    -2.454506     0.323068      25.07
 H      -2.113179    -2.713355     0.204485      27.09
 C       1.626967    -0.724101    -1.482673      63.48
 H       2.285071    -1.045249    -2.250230      23.97
 C       1.573804     0.838280     0.381787      50.95
 H       2.113498     1.588133     0.915508      22.32
 C       0.160901     0.728605     0.534719      33.84
 O      -0.573667     1.526327     1.325846     227.10
 C      -0.024330     2.239513     2.470762     123.51
 H      -0.795990     2.973422     2.930497      26.23
 H       0.299720     1.653312     3.196723      30.13
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 H       0.781394     2.886477     2.263096      27.89
 C      -0.459504    -0.185128    -0.377112      20.32
 O      -1.849522    -0.267519    -0.212564     138.98
 C       0.223140    -1.007182    -1.253659      64.26
 H      -0.268095    -1.994105    -1.950917      20.07
 C       2.398224     0.155105    -0.638366      13.36
 C       3.897987     0.609387    -0.875583      59.31
 H       4.014380     0.211505    -2.103789      20.44
 O       4.031246     2.074667    -0.951032     233.23
 H       4.455428     2.347335    -0.125448      23.78
 C       4.967891    -0.048691     0.114795     102.54
 H       4.919287     0.383137     1.015819      26.82
 O       4.790264    -1.423797     0.292011     309.72
 H       4.903021    -1.865546    -0.635975      28.13
 C       6.446545     0.365104    -0.514900      88.16
 O       6.903934     1.756681    -0.120888     234.49
 H       7.324842     1.452972     0.752478      28.96
 H       6.324690     0.329508    -1.614820      32.64
 H       7.080715    -0.358243    -0.091607      30.78
55
name= lig-ACN-Water-frame_407
 C      -3.106444     0.958911    -3.708353      43.50
 H      -3.404981    -0.020763    -4.226120      18.96
 C      -3.491804     2.182122    -1.702326      60.26
 H      -3.847360     2.177491    -0.716998      23.29
 C      -3.182767     3.505835    -2.312708       2.10
 O      -3.486843     4.785062    -1.686199     195.42
 C      -3.740674     4.812023    -0.248362     117.35
 H      -2.926516     4.404767     0.192732      26.20
 H      -4.625871     4.315093     0.105007      25.80
 H      -4.159308     5.997458     0.151925      23.56
 C      -2.824223     3.444482    -3.726455       4.37
 O      -2.663942     4.588259    -4.509465     148.38
 H      -2.914329     5.531158    -4.043997      15.79
 C      -2.940093     2.180580    -4.382120      48.09
 H      -2.587637     2.295750    -5.368595      27.00
 C      -3.525379     0.973695    -2.301498      38.76
 C      -3.842007    -0.308707    -1.592247      92.34
 H      -4.491433    -0.858480    -2.168720      28.18
 O      -4.782579     0.007927    -0.478260     175.89
 H      -4.287559     0.240291     0.327217      26.69
 C      -2.648704    -1.182448    -1.080744      82.66
 H      -2.059665    -1.467859    -2.086679      24.91
 C      -2.956243    -2.563560    -0.405483     114.71
 O      -3.526077    -3.450361    -1.381743     229.96
 H      -2.953142    -4.000043    -1.908668      28.52
 H      -3.761310    -2.279750     0.502612      24.00
 H      -2.101466    -3.028418    -0.019078      27.50
 C       1.729340    -0.777597    -1.373774      48.09
 H       2.065271    -1.483415    -2.084409      16.97
 C       1.619616     0.839068     0.395761      68.74
 H       2.059964     1.607200     1.095491      17.92
 C       0.228534     0.692979     0.475133       5.42
 O      -0.580801     1.519555     1.316150     202.32
 C       0.026245     2.245558     2.365544     121.22
 H      -0.858214     2.856598     2.780153      24.34
 H       0.359778     1.598894     3.039163      28.15
 H       0.847419     2.817469     1.918341      24.14
 C      -0.521664    -0.274442    -0.328258      11.22
 O      -1.903295    -0.206548    -0.199325     155.23
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 C       0.327277    -0.957400    -1.269680      75.45
 H      -0.257942    -1.974023    -1.875801      19.99
 C       2.335222     0.264194    -0.622213      40.81
 C       3.828868     0.626172    -0.812855      75.99
 H       4.296007     0.180779    -1.930165      20.80
 O       4.027603     2.034431    -0.918313     235.25
 H       4.379634     2.495551    -0.035890      20.03
 C       4.980807     0.030050     0.086647      86.42
 H       4.855431     0.400153     1.025371      25.31
 O       4.855056    -1.431085     0.319820     313.82
 H       4.652411    -1.872467    -0.595033      26.80
 C       6.397282     0.363434    -0.454402      97.33
 O       6.853189     1.702905    -0.085983     284.14
 H       7.189125     1.823603     0.837171      31.16
 H       6.447409     0.458922    -1.591587      31.66
 H       7.155279    -0.385180    -0.308665      30.06
55
name= lig-ACN-Water-frame_408
 C      -3.182862     0.932270    -3.737853      55.53
 H      -3.387161     0.098157    -4.387465      25.85
 C      -3.431266     2.287370    -1.655811      55.50
 H      -4.157195     2.276599    -0.866173      22.76
 C      -3.268282     3.477904    -2.298938      10.56
 O      -3.469794     4.768984    -1.713495     207.95
 C      -3.860567     4.853847    -0.286825     118.76
 H      -3.134073     4.449729     0.339425      26.55
 H      -4.789380     4.363316    -0.070831      25.67
 H      -3.575584     6.063631    -0.152215      23.26
 C      -2.832578     3.458805    -3.701354      -2.28
 O      -2.700222     4.615947    -4.474569     144.22
 H      -3.059775     5.497808    -3.936819      16.78
 C      -2.786589     2.182425    -4.415002      44.78
 H      -2.599746     2.076581    -5.412465      25.25
 C      -3.346560     0.963652    -2.391174       3.90
 C      -3.908811    -0.332489    -1.618321      85.66
 H      -4.396312    -0.919752    -2.390366      26.14
 O      -4.730930    -0.169848    -0.460810     197.62
 H      -4.208721     0.128734     0.276003      27.82
 C      -2.601585    -1.181574    -1.116144      80.29
 H      -1.847644    -1.438731    -1.988659      24.73
 C      -2.883989    -2.577557    -0.382005      97.67
 O      -3.610578    -3.422451    -1.462062     218.54
 H      -2.881741    -3.770980    -1.975919      29.49
 H      -3.671720    -2.581274     0.608958      23.36
 H      -1.947722    -2.945732    -0.068480      27.26
 C       1.744469    -0.814659    -1.305400       6.76
 H       2.461196    -1.388603    -1.852905      18.15
 C       1.605062     0.935842     0.435471      44.03
 H       2.192842     1.651098     1.189339      18.63
 C       0.204085     0.675226     0.475946      18.71
 O      -0.638652     1.453947     1.246922     178.95
 C       0.119971     2.258497     2.294981     119.39
 H      -0.635209     2.947550     2.779308      26.28
 H       0.526042     1.744719     3.025391      29.17
 H       0.845387     3.102004     1.962249      24.29
 C      -0.455800    -0.253646    -0.286615      20.45
 O      -1.921112    -0.272448    -0.227379     171.35
 C       0.358230    -0.973205    -1.188067      79.98
 H      -0.047212    -1.811029    -2.091358      19.27
 C       2.417573     0.219468    -0.605411      18.00
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 C       3.839487     0.561057    -0.818803      68.09
 H       3.910985     0.200082    -2.058711      19.07
 O       4.009137     2.071027    -0.906126     199.06
 H       4.311451     2.358904     0.074078      19.81
 C       4.968030     0.054847     0.140344      92.11
 H       4.942799     0.511870     1.091609      22.95
 O       4.880516    -1.418377     0.321978     301.59
 H       5.107507    -1.843299    -0.574747      27.19
 C       6.365744     0.404234    -0.458394      79.17
 O       6.799600     1.680906    -0.064457     341.17
 H       7.081783     1.446629     0.846269      30.53
 H       6.188625     0.317159    -1.581544      30.21
 H       6.954723    -0.379428     0.081564      28.79
55
name= lig-ACN-Water-frame_409
 C      -3.158322     1.033248    -3.828660      53.49
 H      -2.995501     0.145605    -4.291735      27.86
 C      -3.498440     2.219381    -1.638840      68.62
 H      -3.533313     2.288509    -0.503166      26.20
 C      -3.284262     3.476176    -2.360921      27.57
 O      -3.455786     4.704344    -1.766343     229.02
 C      -3.877118     4.874783    -0.384529     121.61
 H      -3.421554     4.242023     0.363535      26.66
 H      -4.917415     4.724613    -0.364225      28.20
 H      -3.996620     6.057646    -0.126192      25.51
 C      -2.915313     3.457677    -3.709990      18.97
 O      -2.715121     4.565542    -4.438995     185.67
 H      -2.872056     5.551323    -4.011470      20.05
 C      -2.694168     2.207640    -4.379556      39.98
 H      -2.582574     2.363283    -5.394766      21.36
 C      -3.359685     1.013093    -2.291643       3.09
 C      -3.771196    -0.408053    -1.645285      84.19
 H      -4.404508    -1.056417    -2.347973      25.02
 O      -4.706099    -0.287263    -0.468546     110.84
 H      -4.066432     0.056191     0.255307      28.00
 C      -2.606471    -1.197719    -1.155588      92.64
 H      -2.067701    -1.351974    -2.170729      27.60
 C      -2.859432    -2.566417    -0.545365     120.07
 O      -3.615393    -3.360508    -1.446736     200.73
 H      -3.129791    -3.666901    -2.334151      25.51
 H      -3.590088    -2.522265     0.509024      24.56
 H      -1.983579    -3.122629    -0.295530      27.44
 C       1.796352    -0.792520    -1.232795      65.36
 H       2.223585    -1.346828    -2.061783      25.79
 C       1.601711     0.926553     0.371480      72.40
 H       2.099099     1.844894     0.953186      19.62
 C       0.223148     0.738119     0.541278      15.38
 O      -0.623210     1.496870     1.330940     225.18
 C       0.095052     2.318124     2.237422     117.03
 H      -0.640825     2.820950     2.837194      27.33
 H       0.679758     1.698385     2.752860      29.78
 H       0.827456     2.885978     1.469054      23.22
 C      -0.437545    -0.278273    -0.365241      11.91
 O      -1.794678    -0.359002    -0.231444     159.74
 C       0.374129    -1.083194    -1.150986      52.38
 H      -0.240614    -1.893055    -1.861004      19.47
 C       2.399460     0.184950    -0.406894      45.45
 C       3.866355     0.619889    -0.827264      78.72
 H       4.348939     0.153379    -1.923574      23.36
 O       3.971656     2.060075    -0.912930     208.71
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 H       4.336746     2.491213    -0.093366      24.51
 C       4.917865    -0.005065     0.140934     109.05
 H       4.701314     0.423581     1.099885      27.18
 O       4.891749    -1.379402     0.324206     296.58
 H       5.305745    -1.758113    -0.448236      31.89
 C       6.297034     0.342171    -0.421589      91.89
 O       6.771231     1.713165    -0.067066     252.23
 H       7.334598     1.786238     0.706715      27.76
 H       6.507704     0.295088    -1.565231      31.00
 H       7.129614    -0.419924    -0.166849      31.01
55
name= lig-ACN-Water-frame_410
 C      -3.006877     1.043943    -3.634961      45.74
 H      -2.959443     0.211074    -4.194530      21.11
 C      -3.500289     2.198544    -1.629823      51.23
 H      -3.262540     2.099584    -0.487781      23.04
 C      -3.333888     3.379767    -2.296033      10.07
 O      -3.398665     4.711730    -1.803935     227.99
 C      -4.026136     4.877206    -0.514584     130.78
 H      -3.448900     4.211008     0.172048      25.34
 H      -5.069430     4.621242    -0.452429      26.70
 H      -3.571124     5.835487    -0.216897      26.03
 C      -2.977476     3.442043    -3.707230       5.95
 O      -2.700378     4.588402    -4.467373     177.14
 H      -3.130209     5.382936    -3.881077      15.38
 C      -2.747728     2.294124    -4.396127      56.97
 H      -2.158755     2.248826    -5.313252      32.36
 C      -3.518387     0.943550    -2.385342      38.92
 C      -3.706346    -0.354212    -1.612986     101.29
 H      -4.241122    -1.022427    -2.468935      26.10
 O      -4.634429    -0.310523    -0.527612     160.61
 H      -4.317201    -0.036152     0.357776      24.96
 C      -2.425388    -1.213259    -1.275235      83.04
 H      -1.748947    -1.405309    -2.158630      27.57
 C      -2.802714    -2.579330    -0.667615     111.07
 O      -3.696398    -3.359585    -1.494630     200.09
 H      -3.030361    -3.686455    -2.257402      26.80
 H      -3.399785    -2.264704     0.398799      25.09
 H      -1.824168    -3.010585    -0.449939      26.94
 C       1.769101    -0.870861    -1.221008      55.73
 H       2.439254    -1.347139    -1.955427      26.92
 C       1.574300     0.997186     0.430917      54.34
 H       2.006391     1.972107     0.855677      20.30
 C       0.184977     0.708026     0.461406      17.61
 O      -0.661135     1.495763     1.395277     188.31
 C       0.136913     2.405781     2.206723     119.66
 H      -0.523108     2.888967     2.882199      27.90
 H       0.834871     1.985839     2.802350      29.34
 H       0.554505     3.460981     1.753835      24.12
 C      -0.373141    -0.255395    -0.310898      23.85
 O      -1.737091    -0.454056    -0.231489     173.56
 C       0.448506    -1.130562    -1.116846      52.67
 H       0.090049    -1.971476    -1.692758      22.86
 C       2.447670     0.120624    -0.467523      20.74
 C       3.824878     0.605378    -0.762573      79.51
 H       3.813044     0.229308    -1.987268      21.53
 O       3.943666     2.070026    -0.941514     181.56
 H       4.222883     2.393149    -0.111361      27.74
 C       4.952524     0.052713     0.144566      96.95
 H       4.873303     0.481194     1.147800      25.30
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 O       4.866128    -1.432096     0.348224     297.16
 H       4.713768    -1.870064    -0.522316      30.07
 C       6.398295     0.379585    -0.359707      76.87
 O       6.755062     1.753181    -0.121037     270.60
 H       7.088976     1.599068     0.789120      27.75
 H       6.084551     0.316423    -1.446881      29.71
 H       7.101507    -0.410870     0.170358      28.86
55
name= lig-ACN-Water-frame_411
 C      -2.893756     0.980988    -3.662117      53.12
 H      -2.732296     0.075924    -4.161931      23.23
 C      -3.485904     2.153520    -1.591789      45.19
 H      -4.010623     2.203142    -0.524365      19.25
 C      -3.368982     3.427957    -2.353167      10.23
 O      -3.359368     4.695937    -1.823238     250.92
 C      -4.063725     4.846508    -0.567652     126.26
 H      -3.808151     4.119537     0.309329      24.15
 H      -5.123461     4.710199    -0.813359      27.00
 H      -4.067643     5.850124    -0.245618      27.80
 C      -3.012782     3.478908    -3.724761      11.64
 O      -2.732436     4.638115    -4.415845     149.03
 H      -2.984449     5.563698    -4.075019      21.45
 C      -2.758613     2.152899    -4.315054      46.50
 H      -2.296744     2.096202    -5.378888      25.07
 C      -3.539219     0.997947    -2.329741      33.40
 C      -3.673212    -0.376860    -1.709048      90.81
 H      -4.252716    -1.214560    -2.398931      23.83
 O      -4.596399    -0.291148    -0.579400     179.15
 H      -4.057212    -0.030316     0.160689      27.65
 C      -2.294266    -1.168245    -1.375808      80.97
 H      -1.693302    -1.072476    -2.267465      26.77
 C      -2.709381    -2.555294    -0.727588      96.50
 O      -3.738758    -3.383192    -1.566640     155.65
 H      -3.251059    -3.934774    -2.189338      29.68
 H      -3.339413    -2.466470     0.306852      24.60
 H      -1.925401    -3.349177    -0.506051      25.56
 C       1.921000    -0.916293    -1.198849      79.74
 H       2.499813    -1.675761    -1.760644      17.87
 C       1.586018     0.954844     0.371607      75.56
 H       2.074080     1.712184     0.933512      20.05
 C       0.197905     0.821165     0.531501      17.87
 O      -0.614084     1.451604     1.374936     184.87
 C       0.098064     2.566006     2.287290      95.00
 H      -0.670956     2.715717     2.967136      25.79
 H       0.969626     2.208290     2.639356      27.39
 H       0.331861     3.330666     1.379082      23.00
 C      -0.346900    -0.357540    -0.274688      15.17
 O      -1.722785    -0.537964    -0.218934     201.15
 C       0.454207    -1.131541    -1.080317      71.04
 H       0.038250    -1.806303    -1.657019      22.49
 C       2.323957     0.235924    -0.462392      48.81
 C       3.793712     0.574839    -0.770659      60.80
 H       4.275341     0.106827    -1.834194      23.85
 O       3.917332     2.071973    -0.939780     161.68
 H       4.016693     2.537864    -0.055833      25.00
 C       4.996151     0.014137     0.214011      71.86
 H       4.871003     0.500736     1.186938      24.68
 O       4.813374    -1.421897     0.368239     327.22
 H       4.645486    -1.737562    -0.597599      25.20
 C       6.375369     0.403896    -0.383919     105.44
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 O       6.763549     1.788204    -0.129681     258.02
 H       7.349198     1.947491     0.691729      27.51
 H       6.799216     0.123278    -1.386392      30.28
 H       7.197874    -0.253373     0.192191      28.04
55
name= lig-ACN-Water-frame_412
 C      -2.935101     0.902283    -3.636048      46.66
 H      -2.561658    -0.045815    -4.082905      27.11
 C      -3.634679     2.273557    -1.678190      58.49
 H      -4.302934     2.256293    -0.736104      24.20
 C      -3.350454     3.429962    -2.360908      17.35
 O      -3.318929     4.699100    -1.744882     216.95
 C      -4.216694     4.855204    -0.612803     119.53
 H      -3.824591     4.159757     0.266465      25.48
 H      -5.283174     4.573849    -0.853938      26.66
 H      -4.049565     5.790165    -0.357139      29.46
 C      -2.983934     3.381014    -3.760067       7.79
 O      -2.766515     4.648196    -4.393214     129.25
 H      -3.012797     5.256539    -3.717825      25.28
 C      -2.693825     2.179122    -4.337087      42.92
 H      -2.582288     2.270740    -5.517242      12.88
 C      -3.306240     0.944843    -2.322603       4.19
 C      -3.674441    -0.445689    -1.759592      83.84
 H      -4.251861    -1.037308    -2.704832      23.39
 O      -4.540317    -0.283473    -0.617062     189.86
 H      -4.013757    -0.020031     0.228312      25.25
 C      -2.403526    -1.165113    -1.372921      82.82
 H      -1.723666    -1.268250    -2.171870      27.77
 C      -2.720435    -2.671505    -0.901070     112.13
 O      -3.730420    -3.367815    -1.595060     224.56
 H      -3.239167    -3.727809    -2.325635      30.74
 H      -3.088939    -2.292816     0.128873      26.05
 H      -1.648577    -3.138889    -0.753453      24.87
 C       1.854128    -0.919651    -1.114132      -9.82
 H       2.544183    -1.508795    -1.739085      19.86
 C       1.591705     1.027636     0.379000      55.27
 H       2.047318     1.701556     0.971256      22.45
 C       0.220666     0.705514     0.525166      17.42
 O      -0.563079     1.496054     1.466496     220.60
 C      -0.028782     2.578253     2.198873     125.08
 H      -0.632839     2.850075     3.062170      27.19
 H       0.832931     2.404984     2.626741      29.51
 H       0.009528     3.642749     1.626295      25.70
 C      -0.309375    -0.328626    -0.199487      18.32
 O      -1.691817    -0.554626    -0.196337     179.44
 C       0.549891    -1.153877    -1.073292      91.76
 H       0.117812    -1.934558    -1.497140      23.21
 C       2.461341     0.198054    -0.584612      30.06
 C       3.905617     0.637913    -0.717777      89.79
 H       4.064909     0.213922    -1.885264      21.67
 O       3.898232     2.042594    -0.925093     221.90
 H       4.203814     2.519713    -0.001953      21.28
 C       4.935733     0.031782     0.187737     100.58
 H       4.923777     0.383546     1.244545      24.89
 O       4.772184    -1.371940     0.366818     337.93
 H       5.212613    -1.900143    -0.375109      32.14
 C       6.468306     0.379528    -0.293810      74.66
 O       6.774021     1.862519    -0.143934     234.70
 H       7.457810     1.728865     0.593704      27.93
 H       6.328227     0.196164    -1.377184      31.96
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 H       7.162240    -0.286301     0.412623      29.18
55
name= lig-ACN-Water-frame_413
 C      -2.836035     1.003476    -3.702019      46.16
 H      -2.839764    -0.009417    -4.287954      24.19
 C      -3.787439     2.165101    -1.823654      53.69
 H      -4.009767     2.205792    -0.747659      29.72
 C      -3.294328     3.424391    -2.346054       5.48
 O      -3.323262     4.679637    -1.701963     208.70
 C      -4.333624     4.878234    -0.621619     110.52
 H      -3.987299     4.280914     0.353998      24.46
 H      -5.411659     4.522815    -0.933046      24.24
 H      -4.348410     5.793477    -0.366527      29.72
 C      -2.877400     3.419096    -3.699156      12.81
 O      -2.811086     4.560782    -4.364124     148.21
 H      -3.066906     5.405049    -3.956312      22.78
 C      -2.701709     2.135964    -4.446928      78.64
 H      -2.303449     1.970054    -5.560660      23.75
 C      -3.222092     0.993255    -2.309864      15.09
 C      -3.614305    -0.342509    -1.687488      84.27
 H      -4.322265    -1.013169    -2.512282      23.26
 O      -4.551116    -0.304912    -0.641929     152.48
 H      -4.065634    -0.160733     0.218837      25.06
 C      -2.420897    -1.294262    -1.378354      86.14
 H      -1.782675    -1.199359    -2.210874      28.39
 C      -2.700761    -2.658549    -0.894305     128.37
 O      -3.734976    -3.372409    -1.661999     185.04
 H      -3.325338    -3.675706    -2.569599      27.69
 H      -2.969053    -2.942014     0.110721      27.64
 H      -1.774522    -3.373601    -1.140900      23.84
 C       1.955889    -0.887513    -1.139692      44.62
 H       2.467416    -1.580297    -1.819514      23.86
 C       1.683519     1.013382     0.324008      75.65
 H       2.017896     1.915023     0.643485      23.90
 C       0.330388     0.724274     0.617563      -0.21
 O      -0.568435     1.427148     1.473646     176.43
 C      -0.119018     2.648422     2.178209     111.34
 H      -0.953963     2.585047     2.896509      25.24
 H       0.807938     2.571589     2.492843      28.11
 H      -0.217354     3.554532     1.427276      25.84
 C      -0.349930    -0.367189    -0.252082       4.77
 O      -1.736956    -0.545645    -0.186779     138.44
 C       0.462989    -1.176929    -0.959384      59.12
 H       0.117503    -2.047020    -1.541850      22.91
 C       2.503989     0.250459    -0.441033      31.55
 C       3.922965     0.643542    -0.818085      75.40
 H       4.366212     0.194601    -1.872899      22.79
 O       3.940910     2.105694    -0.869831     184.98
 H       4.472495     2.576370    -0.099881      19.35
 C       5.028242     0.111037     0.264833      90.73
 H       4.625797     0.644877     1.162373      25.50
 O       4.769407    -1.365275     0.344903     332.22
 H       5.259669    -1.745194    -0.395802      30.86
 C       6.397123     0.426415    -0.210807     114.22
 O       6.813360     1.819912    -0.124715     298.13
 H       7.220615     2.095844     0.725500      30.64
 H       6.613212     0.154359    -1.256998      30.51
 H       7.264183    -0.257236     0.208212      28.61
55
name= lig-ACN-Water-frame_414
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 C      -2.746311     0.993924    -3.732129      58.84
 H      -2.637107    -0.052849    -4.315186      20.85
 C      -3.712249     2.171306    -1.760379      86.59
 H      -4.266018     2.032524    -0.887110      24.03
 C      -3.322767     3.360978    -2.325837       6.12
 O      -3.392533     4.639339    -1.661540     195.52
 C      -4.399298     4.870555    -0.635075     113.93
 H      -4.276374     4.314637     0.398622      24.17
 H      -5.420817     4.491749    -1.152630      23.49
 H      -4.419083     5.805953    -0.558386      30.25
 C      -2.798735     3.387304    -3.704325       7.87
 O      -2.800527     4.587088    -4.458032     146.82
 H      -3.101304     5.328140    -3.785835      15.19
 C      -2.670455     2.234222    -4.427169      49.89
 H      -2.318951     2.379928    -5.521590      28.28
 C      -3.317431     0.973956    -2.439143      28.06
 C      -3.574142    -0.359850    -1.688693      78.12
 H      -4.120842    -0.966876    -2.670803      23.81
 O      -4.611662    -0.294563    -0.581569     151.51
 H      -4.217245    -0.285039     0.278856      26.30
 C      -2.365041    -1.204317    -1.308554      88.08
 H      -1.750858    -1.362949    -2.160606      26.08
 C      -2.668617    -2.850867    -0.863167      93.06
 O      -3.829042    -3.359144    -1.728728     170.13
 H      -3.169639    -3.791478    -2.480309      25.76
 H      -2.855310    -2.670030     0.139581      28.22
 H      -1.584273    -3.374663    -1.015582      22.77
 C       1.885475    -0.878739    -1.110735      59.59
 H       2.563123    -1.482935    -1.702189      25.95
 C       1.687123     1.084346     0.389068      50.40
 H       2.089034     2.059073     0.639772      19.34
 C       0.286554     0.684576     0.577228      17.95
 O      -0.539180     1.291846     1.408369     184.42
 C      -0.251276     2.663302     2.131703     102.88
 H      -0.870909     2.976783     3.026011      25.25
 H       0.689854     2.674827     2.518361      27.27
 H      -0.368957     3.435338     1.338594      26.37
 C      -0.326656    -0.320878    -0.163440       7.67
 O      -1.778338    -0.535117    -0.188452     177.89
 C       0.597382    -1.184963    -0.934140      70.44
 H       0.081429    -2.034737    -1.598292      20.36
 C       2.527338     0.162474    -0.480004       8.88
 C       3.987106     0.680297    -0.782013      74.60
 H       4.213215     0.307615    -1.910088      20.78
 O       4.004588     2.180745    -0.884684     242.24
 H       4.413160     2.540777    -0.092219      22.49
 C       4.939090     0.128502     0.247121     100.85
 H       4.921263     0.437309     1.359210      21.58
 O       4.841936    -1.284387     0.346724     355.12
 H       4.819776    -1.656420    -0.565789      28.36
 C       6.484367     0.445779    -0.170600      82.68
 O       6.825082     1.824069    -0.082291     301.10
 H       7.289061     1.864529     0.794365      27.87
 H       6.467843     0.139266    -1.199008      33.27
 H       7.068281    -0.164184     0.616170      28.81
55
name= lig-ACN-Water-frame_415
 C      -2.759039     0.966443    -3.758324      49.43
 H      -2.201906     0.045872    -4.237194      23.08
 C      -3.591491     2.129904    -1.694542      46.29
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 H      -4.213338     2.164061    -0.891994      22.19
 C      -3.333380     3.410375    -2.318784      12.36
 O      -3.441745     4.578771    -1.653683     244.60
 C      -4.496449     4.829628    -0.716561     125.11
 H      -4.172730     4.303082     0.250948      24.95
 H      -5.647553     4.552644    -0.959208      24.96
 H      -4.331925     5.769782    -0.392062      28.41
 C      -2.862720     3.511629    -3.687939      -0.75
 O      -2.775404     4.630497    -4.470102     155.48
 H      -2.876528     5.568960    -3.987915      21.13
 C      -2.529581     2.245066    -4.370568      30.91
 H      -2.402699     2.304740    -5.460383      21.71
 C      -3.408522     0.895529    -2.489376      10.57
 C      -3.665790    -0.470144    -1.739216      75.29
 H      -4.252119    -1.393482    -2.363778      21.30
 O      -4.630044    -0.269266    -0.601263     181.59
 H      -4.097731    -0.250675     0.264624      25.49
 C      -2.312510    -1.254188    -1.239922      66.74
 H      -1.616002    -1.078154    -2.047725      24.73
 C      -2.738786    -2.774821    -0.866856     114.70
 O      -3.798511    -3.345517    -1.707803     172.22
 H      -3.494386    -3.840910    -2.519891      28.78
 H      -3.179462    -2.983485    -0.001960      27.83
 H      -1.872172    -3.627393    -0.888175      23.29
 C       1.975272    -0.901953    -1.077083      70.94
 H       2.438131    -1.575315    -1.785276      13.42
 C       1.652376     1.002919     0.359766      61.02
 H       2.020152     1.822598     1.085131      16.29
 C       0.325444     0.718374     0.512307      17.54
 O      -0.622540     1.326695     1.505170     207.28
 C      -0.319821     2.581683     1.987302     130.12
 H      -1.199690     2.484826     2.733246      22.08
 H       0.643897     2.594717     2.414053      25.31
 H      -0.405026     3.404706     1.332921      27.36
 C      -0.281061    -0.422904    -0.175229      19.86
 O      -1.658606    -0.490885    -0.132292     199.75
 C       0.528196    -1.175772    -0.945157     106.70
 H       0.139605    -2.207592    -1.502037      18.20
 C       2.496414     0.328384    -0.474827      45.29
 C       3.899353     0.770134    -0.698685      94.74
 H       4.278743     0.319919    -1.727535      22.72
 O       4.036305     2.157920    -0.927359     278.53
 H       4.290127     2.641180    -0.156475      26.59
 C       5.035171     0.157513     0.226495      71.44
 H       4.627382     0.665647     1.227318      21.70
 O       4.902606    -1.269221     0.327112     336.02
 H       4.779981    -1.728614    -0.583449      27.01
 C       6.471072     0.402321    -0.112506     105.25
 O       6.862828     1.864594    -0.011742     313.24
 H       7.645386     1.964202     0.642532      26.24
 H       6.795203     0.025988    -1.057693      32.92
 H       7.122383    -0.231338     0.534647      29.58
55
name= lig-ACN-Water-frame_416
 C      -2.791281     1.022522    -3.711262      46.21
 H      -2.676099     0.088650    -4.354156      23.77
 C      -3.548967     2.054592    -1.794868      56.05
 H      -3.572058     1.998638    -0.755840      23.04
 C      -3.316948     3.351212    -2.345013       7.29
 O      -3.505709     4.625132    -1.677117     218.76
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 C      -4.510180     4.787850    -0.646698     114.85
 H      -4.515902     4.023578     0.186474      26.44
 H      -5.535179     4.669968    -1.245859      26.07
 H      -4.534353     5.824969    -0.405013      28.40
 C      -2.908886     3.503692    -3.713201       4.77
 O      -2.748905     4.709470    -4.438969     187.81
 H      -2.872651     5.525896    -3.888763      26.02
 C      -2.475452     2.255714    -4.291704      49.50
 H      -1.900919     2.222107    -5.164110      21.47
 C      -3.409570     0.832483    -2.413801      15.11
 C      -3.710418    -0.535265    -1.686718      92.40
 H      -4.254808    -1.224552    -2.562698      23.21
 O      -4.605098    -0.274305    -0.654692     197.48
 H      -4.095184     0.110063     0.144280      25.54
 C      -2.375544    -1.275842    -1.224834      78.05
 H      -1.726118    -1.495613    -2.095858      23.98
 C      -2.814264    -2.705426    -0.810317     111.66
 O      -3.786222    -3.331892    -1.714939     220.69
 H      -3.212627    -3.488103    -2.424906      32.37
 H      -3.103364    -2.500634     0.107492      28.98
 H      -1.761077    -3.275512    -0.867705      23.00
 C       1.965725    -0.856593    -1.074019       6.85
 H       2.752672    -1.348604    -1.616924      18.27
 C       1.584465     1.035807     0.441866      55.59
 H       2.183970     1.808513     1.175463      18.57
 C       0.182036     0.702838     0.569234      24.25
 O      -0.627881     1.224515     1.432509     229.36
 C      -0.389587     2.590308     1.969180     114.48
 H      -1.046376     3.088507     2.748226      25.05
 H       0.583318     2.710959     2.515507      24.77
 H      -0.399345     3.205240     1.150970      27.65
 C      -0.252221    -0.398930    -0.192916      13.57
 O      -1.645201    -0.528593    -0.079184     164.21
 C       0.648175    -1.245476    -0.992984      92.49
 H       0.225756    -2.278825    -1.469687      17.05
 C       2.439508     0.310644    -0.502596      18.01
 C       3.955849     0.728663    -0.767881      84.29
 H       4.121724     0.269513    -1.832386      24.69
 O       4.019212     2.177888    -0.937338     225.74
 H       4.400858     2.684860    -0.169205      21.24
 C       5.020619     0.189850     0.259601      81.41
 H       5.061364     0.511326     1.430882      21.53
 O       4.921340    -1.297660     0.325582     281.06
 H       5.194965    -1.558455    -0.619863      29.53
 C       6.566529     0.482278    -0.059277      97.67
 O       6.905250     1.839047    -0.000367     300.31
 H       7.456079     2.017854     0.890037      25.28
 H       6.668364     0.162255    -1.064892      31.78
 H       7.066034    -0.098098     0.689249      29.79
55
name= lig-ACN-Water-frame_417
 C      -2.863763     0.958130    -3.716277      66.57
 H      -2.776478     0.143877    -4.392615      27.28
 C      -3.499765     2.116435    -1.702667      56.90
 H      -3.580853     2.150382    -0.605486      23.47
 C      -3.389138     3.368244    -2.365094      -5.63
 O      -3.509239     4.617584    -1.696608     197.44
 C      -4.587005     4.738242    -0.656434     115.59
 H      -4.543451     3.968994     0.109495      25.68
 H      -5.623652     4.720829    -1.160140      25.75
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 H      -4.263002     5.595045     0.012690      26.29
 C      -2.888950     3.484598    -3.742833      10.42
 O      -2.724049     4.710166    -4.358721     206.21
 H      -2.911026     5.377230    -3.723877      26.85
 C      -2.438222     2.272024    -4.269584      42.00
 H      -1.808864     2.356514    -5.058492      21.04
 C      -3.301793     0.852043    -2.431511      25.35
 C      -3.609228    -0.407946    -1.731520      91.08
 H      -4.194690    -1.172245    -2.476733      23.62
 O      -4.627618    -0.312682    -0.632418     117.89
 H      -4.317063     0.305495     0.009870      29.49
 C      -2.470277    -1.276321    -1.270738      89.61
 H      -1.745931    -1.199487    -2.136674      25.61
 C      -2.817562    -2.629627    -0.652223     115.12
 O      -3.725121    -3.295935    -1.688083     174.68
 H      -3.240133    -3.655687    -2.462057      28.92
 H      -3.405952    -2.725890     0.154160      28.30
 H      -1.934874    -3.367906    -0.417631      25.56
 C       2.007448    -0.807047    -1.136045      56.11
 H       2.617292    -1.530537    -1.667281      22.82
 C       1.598195     1.044084     0.477340      68.27
 H       1.894655     2.158932     0.977988      18.70
 C       0.306321     0.617393     0.550509      -1.15
 O      -0.732841     1.208789     1.497848     147.39
 C      -0.378756     2.664740     1.904742     101.95
 H      -1.324381     2.775601     2.471046      25.32
 H       0.623203     2.527025     2.505472      23.68
 H      -0.238831     3.254008     1.138691      30.31
 C      -0.267084    -0.433713    -0.292913      -9.58
 O      -1.740680    -0.683905    -0.148841     140.51
 C       0.662790    -1.257286    -0.942555      52.69
 H       0.324573    -2.177928    -1.533723      21.99
 C       2.450200     0.322606    -0.411052      24.54
 C       3.955650     0.691974    -0.747539      86.78
 H       4.351971     0.289192    -1.711596      25.90
 O       3.994560     2.169002    -0.962411     204.20
 H       4.245455     2.646066    -0.027733      22.01
 C       5.053164     0.122750     0.292662      82.68
 H       4.476440     0.532709     1.330876      23.17
 O       4.949338    -1.274861     0.324193     333.35
 H       5.103556    -1.692967    -0.550171      28.66
 C       6.554134     0.484172    -0.049338     111.03
 O       6.921368     1.900497    -0.039071     267.32
 H       7.717216     1.982455     0.707094      24.13
 H       6.813330     0.111419    -1.011015      32.07
 H       7.205368    -0.064934     0.551118      29.77
55
name= lig-ACN-Water-frame_418
 C      -2.818066     0.995109    -3.836457      47.49
 H      -2.545788     0.098707    -4.206549      24.73
 C      -3.418442     2.206699    -1.638550      69.21
 H      -3.996732     2.158777    -0.640667      21.84
 C      -3.449800     3.410014    -2.351525      28.97
 O      -3.562231     4.602470    -1.686535     250.98
 C      -4.568806     4.664302    -0.664564     121.25
 H      -4.598704     3.741365    -0.177880      25.59
 H      -5.589521     4.973528    -0.971485      26.76
 H      -4.260452     5.629191    -0.009468      25.32
 C      -2.872590     3.458404    -3.618639       7.42
 O      -2.689389     4.650513    -4.277052     205.12
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 H      -2.777947     5.561202    -3.830248      22.54
 C      -2.444966     2.201968    -4.350282      39.56
 H      -2.193500     2.221934    -5.348220      22.02
 C      -3.252404     1.054413    -2.344695       6.84
 C      -3.653477    -0.367986    -1.710036      86.73
 H      -4.152748    -0.983529    -2.589335      25.09
 O      -4.653948    -0.316848    -0.656703     148.84
 H      -4.324343     0.221883     0.115673      26.02
 C      -2.398727    -1.290555    -1.258022      86.88
 H      -1.840588    -1.700693    -2.157188      24.44
 C      -2.947412    -2.667533    -0.652705     113.94
 O      -3.659147    -3.321660    -1.628108     203.33
 H      -2.911012    -3.682111    -2.308679      25.79
 H      -3.534984    -2.271978     0.110286      27.00
 H      -1.975140    -3.127838    -0.265995      25.28
 C       1.978692    -0.819756    -1.086503      46.18
 H       2.648779    -1.246621    -1.846179      22.31
 C       1.630066     1.010141     0.419151      62.55
 H       1.917949     2.149271     0.903881      17.50
 C       0.188146     0.559482     0.597781       5.97
 O      -0.639388     1.242792     1.452215     224.97
 C      -0.409705     2.570913     1.840717     122.19
 H      -1.223373     3.033913     2.353296      26.80
 H       0.376540     2.771818     2.773948      23.15
 H      -0.190979     3.167167     1.116254      29.70
 C      -0.371706    -0.469082    -0.247386      14.65
 O      -1.658362    -0.737780    -0.184257     199.60
 C       0.612492    -1.235659    -0.993212      56.10
 H       0.316513    -2.098847    -1.536035      22.81
 C       2.588851     0.291551    -0.393071      20.42
 C       3.964796     0.729376    -0.684036      99.55
 H       4.070076     0.300796    -1.675673      21.25
 O       3.991117     2.111273    -0.959118     245.27
 H       4.090411     2.765667    -0.093482      19.01
 C       5.025206     0.154157     0.277474      83.41
 H       4.984116     0.553995     1.499971      20.34
 O       4.967605    -1.322227     0.346834     321.27
 H       4.907662    -1.549059    -0.601316      26.73
 C       6.517847     0.478731    -0.049425     103.77
 O       6.900366     1.966572    -0.122595     279.82
 H       7.614441     2.168392     0.692276      26.43
 H       6.626071     0.098156    -1.049883      32.67
 H       7.042234    -0.002393     0.654640      30.89
55
name= lig-ACN-Water-frame_419
 C      -2.743076     1.037085    -3.620776      70.86
 H      -2.686192     0.182721    -4.165674      24.69
 C      -3.480899     2.210965    -1.640612      58.32
 H      -3.853403     2.060683    -0.519290      20.91
 C      -3.344447     3.432693    -2.291202      18.80
 O      -3.641628     4.680088    -1.700498     238.23
 C      -4.576940     4.667135    -0.611330     117.09
 H      -4.849349     3.816690    -0.089673      26.36
 H      -5.453921     4.999622    -1.129371      26.55
 H      -4.109837     5.347457     0.302406      24.55
 C      -2.793556     3.408171    -3.640881       4.17
 O      -2.626245     4.608562    -4.281307     186.52
 H      -2.814293     5.363590    -3.574845      17.83
 C      -2.604842     2.303508    -4.414991      61.74
 H      -2.210543     2.450839    -5.438411      26.32
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 C      -3.204977     0.989848    -2.370440      45.76
 C      -3.600033    -0.330576    -1.719516      95.46
 H      -4.176344    -0.836448    -2.555302      24.58
 O      -4.663827    -0.267939    -0.706178     163.69
 H      -4.227015    -0.065092     0.207362      24.19
 C      -2.426219    -1.380392    -1.281229      69.50
 H      -1.678493    -1.445555    -2.120585      22.34
 C      -2.999964    -2.547599    -0.611656     110.94
 O      -3.649054    -3.475963    -1.633911     185.57
 H      -3.003761    -3.642600    -2.447433      26.80
 H      -3.792465    -2.470949     0.183429      24.93
 H      -2.292336    -3.215867    -0.105331      25.12
 C       1.954058    -0.853377    -1.055638      40.52
 H       2.519038    -1.411883    -1.816326      19.69
 C       1.515581     0.932386     0.403352      71.00
 H       2.028458     1.793547     1.119104      20.52
 C       0.290110     0.590913     0.544578      31.18
 O      -0.625545     1.232515     1.415559     227.99
 C      -0.401335     2.621676     1.829062     119.56
 H      -1.386884     2.884340     2.040135      26.47
 H       0.506757     2.532532     2.664617      22.35
 H      -0.015011     3.089230     1.083241      29.62
 C      -0.229001    -0.498957    -0.159483       6.74
 O      -1.642458    -0.713938    -0.150502     148.89
 C       0.608983    -1.165263    -1.072514      82.89
 H       0.237008    -1.887271    -1.644484      21.61
 C       2.454037     0.190195    -0.366704      41.08
 C       3.975828     0.691700    -0.668747      91.53
 H       4.367133     0.288919    -1.538255      26.26
 O       4.013363     2.153261    -0.931396     220.44
 H       4.316878     2.625089    -0.073171      22.90
 C       5.077681     0.200860     0.327896      77.48
 H       4.743462     0.539169     1.548610      21.86
 O       4.958000    -1.311621     0.356414     309.88
 H       5.156745    -1.661710    -0.576522      28.80
 C       6.507560     0.572272    -0.109833     122.43
 O       6.846371     1.949315    -0.183154     280.85
 H       7.207069     2.190328     0.726658      28.13
 H       6.829027     0.106709    -1.054076      32.73
 H       7.125059     0.131969     0.540512      31.97
55
name= lig-ACN-Water-frame_422
 C      -2.731995     1.082575    -3.671084      63.51
 H      -2.781683     0.058188    -4.262525      21.38
 C      -3.406876     2.235993    -1.611649      70.59
 H      -3.963924     2.276789    -0.730916      21.47
 C      -3.362429     3.498740    -2.266969      10.26
 O      -3.703411     4.686939    -1.652327     230.54
 C      -4.577413     4.819466    -0.558186     110.08
 H      -4.965269     3.763216    -0.399728      23.40
 H      -5.285115     5.592841    -0.680307      25.85
 H      -3.969732     5.399155     0.433882      23.14
 C      -2.765278     3.601924    -3.571528       7.12
 O      -2.491155     4.718423    -4.318130     178.52
 H      -2.492581     5.562894    -3.734645      20.08
 C      -2.555071     2.314620    -4.215874      38.63
 H      -2.238305     2.345937    -5.359221      24.95
 C      -3.146455     1.003790    -2.266100       4.39
 C      -3.565317    -0.381319    -1.675928      90.39
 H      -4.056970    -0.885671    -2.412041      28.93
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 O      -4.598960    -0.165817    -0.662449     159.75
 H      -4.351608     0.403846     0.159405      23.40
 C      -2.471880    -1.464110    -1.173690      84.55
 H      -1.902371    -1.841932    -2.041831      24.83
 C      -2.989685    -2.829751    -0.548941      94.64
 O      -3.633431    -3.738235    -1.613374     136.25
 H      -2.903140    -3.934934    -2.398062      26.04
 H      -3.969484    -2.559315     0.158185      22.86
 H      -2.129523    -3.141266    -0.086021      26.00
 C       1.909359    -0.849762    -1.206772      60.34
 H       2.543055    -1.224644    -2.019696      22.30
 C       1.660875     0.790047     0.492276      55.76
 H       1.939814     1.543602     1.142181      21.48
 C       0.194400     0.537379     0.596117       7.14
 O      -0.695654     1.287712     1.292430     192.93
 C      -0.260066     2.614918     1.705586     122.85
 H      -1.106550     3.139839     2.067823      26.90
 H       0.250997     2.727678     2.810515      23.41
 H       0.173235     3.272559     1.107308      29.15
 C      -0.279070    -0.443113    -0.310452      18.16
 O      -1.715901    -0.630733    -0.071612     108.07
 C       0.538417    -1.200782    -1.015725      68.54
 H       0.301842    -2.169018    -1.606498      22.24
 C       2.515988     0.171238    -0.403176      22.07
 C       4.004356     0.648537    -0.717297      85.37
 H       4.209113     0.420241    -1.685556      23.61
 O       3.973391     2.144670    -0.847716     222.33
 H       4.390013     2.680139    -0.104573      22.55
 C       5.075332     0.211230     0.275456      68.99
 H       4.811325     0.807389     1.423104      21.05
 O       5.043439    -1.266679     0.479810     317.83
 H       5.093675    -1.590018    -0.429210      29.19
 C       6.477056     0.671427    -0.246032     106.85
 O       6.743309     2.059805    -0.208043     282.21
 H       7.231628     2.321524     0.703183      27.65
 H       6.645770     0.219921    -1.296827      30.75
 H       7.144637     0.227720     0.491698      28.52
55
name= lig-ACN-Water-frame_423
 C      -2.764593     1.155886    -3.621534      53.90
 H      -2.808224     0.295365    -4.419490      20.49
 C      -3.440829     2.258613    -1.609446      54.25
 H      -3.368729     2.268835    -0.608496      23.25
 C      -3.385167     3.463899    -2.324268       5.94
 O      -3.641131     4.738844    -1.689932     179.34
 C      -4.610759     4.885485    -0.477188      88.46
 H      -5.292170     3.959790    -0.161671      24.56
 H      -5.379384     5.628603    -0.703687      24.89
 H      -3.791088     4.887198     0.497004      22.48
 C      -2.694507     3.543283    -3.587345       5.93
 O      -2.507502     4.699817    -4.260388     195.98
 H      -2.558389     5.680964    -3.833367      17.21
 C      -2.440334     2.398684    -4.291347      54.74
 H      -1.770367     2.401482    -5.183615      25.15
 C      -3.140081     1.051403    -2.292225      32.31
 C      -3.619164    -0.407736    -1.640873      94.48
 H      -4.120786    -0.809477    -2.397601      28.43
 O      -4.622817    -0.210016    -0.574880     170.44
 H      -4.089297     0.185301     0.228423      22.18
 C      -2.533713    -1.410122    -1.194330      76.00
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 H      -1.822238    -1.546175    -2.019733      23.40
 C      -2.947989    -2.878969    -0.529448     100.48
 O      -3.555622    -3.716211    -1.555302     200.08
 H      -2.947369    -3.702149    -2.436326      25.49
 H      -3.735749    -2.718025     0.417658      23.03
 H      -2.200339    -3.425130    -0.091667      25.92
 C       1.923359    -0.805766    -1.266307      49.56
 H       2.412543    -1.493632    -1.947354      23.84
 C       1.591685     0.816839     0.571444      67.48
 H       2.012767     1.366830     1.246070      23.05
 C       0.256996     0.556910     0.482561      21.03
 O      -0.649460     1.321581     1.247392     198.33
 C      -0.255534     2.656397     1.741302     100.19
 H      -1.256000     3.019082     1.925898      24.71
 H       0.559585     2.407652     2.599107      22.88
 H       0.238352     3.064592     0.910347      27.12
 C      -0.414662    -0.493093    -0.161074      10.32
 O      -1.712706    -0.739154    -0.151319     162.55
 C       0.582712    -1.216086    -1.018300      49.05
 H      -0.046063    -1.991928    -1.681394      19.81
 C       2.510860     0.180036    -0.430876      19.44
 C       3.883822     0.647872    -0.730268      95.11
 H       4.128037     0.162155    -1.655540      24.96
 O       3.917052     2.144451    -0.917045     179.66
 H       4.158290     2.627191     0.032996      20.38
 C       5.069024     0.169631     0.223119      77.44
 H       4.853147     0.652349     1.429044      22.00
 O       5.070182    -1.202432     0.483157     293.69
 H       5.390391    -1.679112    -0.319868      29.15
 C       6.524942     0.665758    -0.209959      93.87
 O       6.739458     2.128383    -0.184037     260.09
 H       7.397661     2.297462     0.628952      25.06
 H       6.573819     0.472492    -1.357405      29.38
 H       7.358967     0.027509     0.191921      29.59
55
name= lig-ACN-Water-frame_424
 C      -2.771092     1.138344    -3.680725      45.98
 H      -2.392618     0.125428    -4.024480      24.78
 C      -3.404845     2.259956    -1.573821      57.21
 H      -3.655869     2.321990    -0.548935      22.93
 C      -3.350880     3.543297    -2.249487      10.53
 O      -3.653507     4.779840    -1.703010     181.71
 C      -4.539184     4.817212    -0.484354      97.45
 H      -5.313583     3.919330    -0.555414      24.21
 H      -4.856041     5.918025    -0.640524      24.39
 H      -3.924778     5.123653     0.569165      23.33
 C      -2.747199     3.585590    -3.594632      -9.54
 O      -2.490695     4.770115    -4.262619     183.65
 H      -2.710912     5.457292    -3.577076      23.59
 C      -2.292140     2.357291    -4.261095      44.61
 H      -1.915074     2.465217    -5.230971      19.89
 C      -3.235729     0.993441    -2.286506       2.95
 C      -3.715809    -0.371120    -1.648314     101.83
 H      -4.214702    -0.908711    -2.323589      28.81
 O      -4.597110    -0.262624    -0.557838     195.26
 H      -4.249701     0.271550     0.241773      22.22
 C      -2.489603    -1.413504    -1.182845      91.09
 H      -1.974157    -1.580562    -2.142773      26.14
 C      -2.893399    -2.813187    -0.603717     108.23
 O      -3.514008    -3.683232    -1.497998     238.35
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 H      -2.953025    -3.769057    -2.284238      30.71
 H      -3.670020    -2.735628     0.315300      23.63
 H      -1.922645    -3.099043    -0.331055      26.13
 C       1.848788    -0.846699    -1.214966      36.57
 H       2.566085    -1.167964    -1.953158      19.60
 C       1.690706     0.802314     0.536314      59.67
 H       2.008829     1.542494     1.049515      20.00
 C       0.203658     0.625455     0.533470     -14.22
 O      -0.679386     1.360833     1.243946     200.13
 C      -0.237259     2.609777     1.710557     118.76
 H      -0.967117     3.306433     2.218147      24.57
 H       0.520590     2.687586     2.647467      23.14
 H       0.215787     3.302115     0.990389      25.73
 C      -0.251088    -0.605154    -0.210135      -2.90
 O      -1.804925    -0.808295    -0.117859     152.81
 C       0.514055    -1.247024    -1.095315      78.41
 H       0.300871    -2.110377    -1.853615      20.22
 C       2.390274     0.172019    -0.426592      26.03
 C       3.868125     0.687103    -0.736741      75.26
 H       4.141684     0.315214    -1.786840      23.72
 O       3.874106     2.084551    -0.994900     207.57
 H       4.027032     2.641965    -0.070257      20.84
 C       5.103591     0.253799     0.241140      63.36
 H       4.858973     0.800942     1.392687      21.21
 O       5.105556    -1.217477     0.465468     296.98
 H       5.382449    -1.645249    -0.440214      27.52
 C       6.488342     0.682621    -0.303180      89.95
 O       6.754715     2.163773    -0.122445     261.56
 H       7.439941     2.358513     0.583183      26.52
 H       6.574974     0.413894    -1.421423      30.05
 H       7.275505     0.126147     0.361536      28.57
55
name= lig-ACN-Water-frame_425
 C      -2.657465     1.032215    -3.586543      50.29
 H      -2.431687     0.205035    -4.242822      23.43
 C      -3.423406     2.265360    -1.588767      56.37
 H      -4.141332     2.179822    -0.751807      20.86
 C      -3.205211     3.515896    -2.233351      -3.46
 O      -3.648728     4.787099    -1.694661     196.03
 C      -4.418060     4.867462    -0.573207     110.73
 H      -5.381808     4.116448    -0.637788      24.52
 H      -5.101653     5.812975    -0.368807      24.30
 H      -3.847340     4.264353     0.374657      23.04
 C      -2.764659     3.598342    -3.581793      17.70
 O      -2.500389     4.799493    -4.238948     181.13
 H      -2.479742     5.706330    -3.932639      24.75
 C      -2.352771     2.324309    -4.111779      35.01
 H      -1.950966     2.290576    -5.030361      20.15
 C      -3.344925     1.053969    -2.328729       8.52
 C      -3.682273    -0.412934    -1.689957      94.56
 H      -4.210495    -0.861555    -2.439679      27.44
 O      -4.634343    -0.259921    -0.558211     140.76
 H      -4.152620     0.235493     0.126703      25.30
 C      -2.527552    -1.352310    -1.296459      61.62
 H      -1.746664    -1.520749    -2.048229      24.42
 C      -2.785376    -2.680931    -0.642492     107.99
 O      -3.534950    -3.703964    -1.513969     203.81
 H      -2.926847    -3.961296    -2.219706      29.98
 H      -3.409846    -2.484532     0.308260      24.00
 H      -1.918599    -3.212464    -0.232679      24.01
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 C       1.898611    -0.904180    -1.226911      32.83
 H       2.397145    -1.356517    -2.080736      22.09
 C       1.559227     0.893298     0.526450      55.00
 H       1.991855     1.714681     0.921339      20.21
 C       0.226995     0.491002     0.576606      11.90
 O      -0.754283     1.373216     1.255006     148.90
 C      -0.175855     2.705990     1.759510      81.75
 H      -1.200506     2.955607     2.125342      24.15
 H       0.663895     2.366259     2.521772      22.48
 H       0.210736     3.334219     0.848467      24.71
 C      -0.395752    -0.539246    -0.205692     -10.48
 O      -1.661567    -0.771786    -0.012778      92.32
 C       0.515540    -1.338960    -1.207246      60.11
 H       0.019952    -2.179702    -1.733144      17.93
 C       2.486914     0.159302    -0.427512      19.52
 C       3.893944     0.617219    -0.745790      82.30
 H       4.154733     0.066230    -1.767541      21.99
 O       3.829830     2.109682    -1.046837     205.39
 H       4.301222     2.599824    -0.315304      21.13
 C       5.049384     0.290813     0.209208      83.61
 H       5.006514     0.816925     1.375181      19.77
 O       5.140156    -1.178806     0.417087     296.16
 H       5.103401    -1.555673    -0.513005      26.85
 C       6.451323     0.794723    -0.318627      87.51
 O       6.731419     2.141229    -0.156091     319.77
 H       7.174228     2.240261     0.689000      28.63
 H       6.645778     0.460259    -1.386241      30.39
 H       7.195993     0.073836     0.314389      28.37
55
name= lig-ACN-Water-frame_426
 C      -2.598292     1.072720    -3.456542      63.63
 H      -2.581961     0.195722    -4.010668      23.70
 C      -3.606838     2.249072    -1.679546      49.89
 H      -4.071248     2.309339    -0.605106      20.89
 C      -3.185878     3.553919    -2.178975       6.91
 O      -3.544204     4.798862    -1.793768     175.49
 C      -4.451942     4.738492    -0.523127      88.75
 H      -5.485480     4.233344    -0.835370      22.86
 H      -4.209934     5.888554    -0.264978      22.93
 H      -3.785233     4.319898     0.406760      23.15
 C      -2.634917     3.588939    -3.477411      -0.60
 O      -2.507307     4.729974    -4.293017     203.23
 H      -2.529795     5.412721    -3.642214      21.81
 C      -2.432808     2.346290    -4.106722      66.11
 H      -1.886044     2.421532    -4.958382      30.31
 C      -3.291180     0.969020    -2.287153      39.89
 C      -3.691218    -0.351147    -1.705212     104.14
 H      -4.145516    -1.010628    -2.389338      28.64
 O      -4.636750    -0.238509    -0.631137     156.83
 H      -4.243822    -0.014977     0.212927      25.31
 C      -2.400860    -1.231530    -1.312271      60.46
 H      -1.782825    -1.036069    -2.210798      26.01
 C      -2.805814    -2.708263    -0.688323     100.44
 O      -3.532189    -3.657160    -1.478540     177.82
 H      -2.898418    -3.876789    -2.321475      26.50
 H      -3.469683    -2.504445     0.158490      25.30
 H      -1.759551    -3.120184    -0.447987      23.96
 C       1.897060    -0.938938    -1.245633      48.70
 H       2.618025    -1.544752    -1.785290      24.29
 C       1.556602     0.851878     0.356896      54.38
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 H       1.812173     1.712338     0.990351      22.76
 C       0.182718     0.500730     0.609757       8.38
 O      -0.725082     1.346727     1.241096     173.07
 C      -0.238992     2.624447     1.790055     100.50
 H      -0.836134     3.331238     2.437703      24.52
 H       0.674052     2.637307     2.509301      24.52
 H       0.135326     3.316542     0.847142      25.73
 C      -0.290040    -0.528583    -0.288361       8.18
 O      -1.692024    -0.733579    -0.018629     148.76
 C       0.514253    -1.248301    -1.059433      78.55
 H       0.182595    -1.949324    -1.726860      25.99
 C       2.420058     0.088747    -0.416674      20.86
 C       3.867321     0.625391    -0.777288      74.02
 H       4.207118     0.085339    -1.820619      24.03
 O       3.816599     2.093349    -1.090446     224.05
 H       4.244448     2.552416    -0.405856      25.65
 C       5.050260     0.270232     0.168719      98.32
 H       4.618946     0.687044     1.267190      23.31
 O       5.141459    -1.099036     0.343982     340.94
 H       5.255204    -1.589904    -0.470909      30.51
 C       6.410348     0.731841    -0.308828      94.45
 O       6.683716     2.206678    -0.220866     211.97
 H       7.249297     2.482879     0.489613      25.44
 H       6.373515     0.547951    -1.406568      32.39
 H       7.351522     0.126338     0.206338      29.61
55
name= lig-ACN-Water-frame_427
 C      -2.610230     1.119106    -3.506473      52.99
 H      -2.137882     0.289990    -3.932428      26.56
 C      -3.739105     2.280973    -1.667540      70.42
 H      -4.224899     2.211530    -0.583505      22.05
 C      -3.255377     3.471666    -2.245078       7.90
 O      -3.525502     4.779797    -1.711041     221.56
 C      -4.312687     4.753658    -0.526530     104.04
 H      -5.478984     4.623552    -0.799996      24.39
 H      -4.511488     5.858594    -0.050266      23.15
 H      -4.105017     3.866649     0.195041      24.68
 C      -2.526706     3.515785    -3.484169      11.46
 O      -2.491583     4.615707    -4.268850     167.95
 H      -2.694977     5.596412    -4.038549      19.26
 C      -2.333131     2.310353    -4.163061      54.91
 H      -2.154642     2.322223    -5.222432      23.26
 C      -3.250840     1.074373    -2.169513       3.04
 C      -3.630466    -0.355748    -1.648168     101.80
 H      -4.079409    -0.826152    -2.513655      25.96
 O      -4.673860    -0.226516    -0.664991     171.40
 H      -4.208101     0.084918     0.199187      24.32
 C      -2.395516    -1.178196    -1.232795      96.94
 H      -1.672233    -1.454542    -2.026151      23.99
 C      -2.763429    -2.649841    -0.762454     107.18
 O      -3.531758    -3.608992    -1.492156     195.70
 H      -3.071576    -3.764750    -2.451455      26.70
 H      -3.292793    -2.525835     0.140061      26.23
 H      -1.754580    -3.169837    -0.352270      23.41
 C       1.935429    -1.003128    -1.150921       9.03
 H       2.478976    -1.622662    -1.885494      17.64
 C       1.572353     0.839581     0.341630      65.99
 H       2.237908     1.725768     0.743617      17.96
 C       0.209280     0.637369     0.505787      24.48
 O      -0.690835     1.317501     1.297865     219.23
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 C      -0.234799     2.565709     1.797622      94.26
 H      -1.212954     2.723642     2.277468      22.38
 H       0.699033     2.328713     2.408811      24.11
 H      -0.017661     3.425317     0.876612      23.20
 C      -0.350765    -0.459730    -0.142392       1.80
 O      -1.735376    -0.677611    -0.161253     201.96
 C       0.537895    -1.278814    -1.057014     104.76
 H       0.166461    -2.067246    -1.602251      19.82
 C       2.457189     0.126406    -0.495434      36.04
 C       3.814754     0.659919    -0.844290      85.09
 H       4.015180     0.223903    -1.969733      21.82
 O       3.803566     2.041039    -1.122069     223.14
 H       3.918053     2.553356    -0.265189      24.50
 C       4.985594     0.310349     0.185743      83.64
 H       4.924666     0.797176     1.295987      22.92
 O       5.116820    -1.167678     0.299774     281.70
 H       5.511720    -1.406095    -0.584095      29.91
 C       6.392353     0.797122    -0.372687      84.96
 O       6.626982     2.257093    -0.292621     262.26
 H       7.215949     2.242418     0.475946      27.16
 H       6.523839     0.422750    -1.406326      32.06
 H       7.232327     0.162606     0.316841      29.36
55
name= lig-ACN-Water-frame_428
 C      -2.582663     1.072895    -3.464636      59.99
 H      -2.401098     0.052423    -3.814461      26.04
 C      -3.732142     2.294956    -1.612897      42.89
 H      -4.647106     2.325291    -0.907163      20.16
 C      -3.339016     3.500257    -2.258534       2.04
 O      -3.473739     4.717776    -1.643745     219.81
 C      -4.349258     4.795668    -0.499558      87.21
 H      -5.462380     4.628892    -0.858531      22.00
 H      -3.931363     5.725697     0.116674      23.46
 H      -4.016651     4.003736     0.233494      24.88
 C      -2.615054     3.459082    -3.533571     -13.39
 O      -2.425131     4.602672    -4.315503     134.99
 H      -2.592442     5.396860    -3.637802      24.16
 C      -2.231887     2.256814    -4.193733      49.29
 H      -1.882984     2.236690    -5.295239      19.17
 C      -3.199741     1.115656    -2.256113      35.44
 C      -3.564959    -0.276738    -1.674552      80.06
 H      -4.141765    -0.860026    -2.467060      25.61
 O      -4.689446    -0.225013    -0.630854     138.65
 H      -4.361509     0.063898     0.305129      23.18
 C      -2.459268    -1.311985    -1.311779      65.03
 H      -1.877154    -1.211800    -2.252957      23.16
 C      -2.738146    -2.643141    -0.632485     101.95
 O      -3.566363    -3.543615    -1.575496     200.93
 H      -2.948081    -3.717965    -2.312369      30.69
 H      -3.254436    -2.515103     0.268683      24.95
 H      -1.629417    -3.177715    -0.631758      19.29
 C       1.905939    -1.075738    -1.098682      34.47
 H       2.491004    -1.560723    -1.907131      16.64
 C       1.686840     0.956117     0.381798      55.75
 H       1.892265     2.020173     0.953633      12.12
 C       0.250459     0.664407     0.408318       3.25
 O      -0.647540     1.257837     1.304506     198.23
 C      -0.303674     2.543442     1.884362      98.44
 H      -0.957752     3.053463     2.602681      23.21
 H       0.606040     2.558645     2.550554      23.62
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 H      -0.051906     3.393926     0.933389      21.41
 C      -0.342010    -0.524367    -0.232283      12.21
 O      -1.706598    -0.504767    -0.151422     138.75
 C       0.480379    -1.335761    -0.957455     106.19
 H       0.011685    -2.224512    -1.401200      20.54
 C       2.444871     0.124304    -0.553306      31.63
 C       3.852380     0.627251    -0.865321      76.59
 H       4.309471    -0.008679    -1.820895      23.12
 O       3.767430     2.108753    -1.134565     153.10
 H       4.058707     2.659442    -0.232361      19.49
 C       4.998606     0.276408     0.072273      80.71
 H       4.668838     0.656981     1.124737      24.78
 O       5.092501    -1.176821     0.280440     290.92
 H       5.101074    -1.711487    -0.635905      27.75
 C       6.343028     0.855375    -0.407381      95.11
 O       6.582290     2.249710    -0.331389     245.00
 H       7.216387     2.605367     0.389224      27.31
 H       6.594531     0.537956    -1.437810      32.51
 H       7.170523     0.355399     0.382246      28.28
55
name= lig-ACN-Water-frame_429
 C      -2.476471     0.995173    -3.471687      53.36
 H      -2.433078     0.057746    -4.121903      21.15
 C      -3.666326     2.267494    -1.718004      82.56
 H      -4.315199     2.152946    -0.830597      21.02
 C      -3.329341     3.478069    -2.311910      11.92
 O      -3.418985     4.722152    -1.655399     178.37
 C      -4.334188     4.799826    -0.397906     104.93
 H      -5.467125     4.997605    -0.627648      24.92
 H      -4.144242     5.872871    -0.131872      24.66
 H      -4.201113     4.044843     0.304635      27.43
 C      -2.738111     3.447853    -3.623715       3.05
 O      -2.356084     4.619621    -4.303962     176.28
 H      -2.407677     5.511896    -3.884895      22.16
 C      -2.247576     2.200557    -4.121263      15.39
 H      -1.401402     2.322212    -4.962680      20.23
 C      -3.273459     1.039274    -2.218563      12.76
 C      -3.745039    -0.303779    -1.651159      95.62
 H      -4.267160    -0.815529    -2.568591      23.43
 O      -4.636291    -0.200025    -0.591676     207.34
 H      -4.105064    -0.040801     0.190147      25.90
 C      -2.455937    -1.185243    -1.273801      71.56
 H      -1.749187    -1.531757    -2.037205      22.28
 C      -2.786041    -2.733547    -0.645636      99.22
 O      -3.563269    -3.418142    -1.600728     233.03
 H      -2.924394    -3.752985    -2.199454      30.98
 H      -3.295676    -2.632789     0.318215      24.98
 H      -1.705927    -3.253576    -0.280612      22.04
 C       1.835516    -1.019739    -1.070217      67.23
 H       2.489834    -1.753508    -1.591934      22.07
 C       1.627510     0.977116     0.297032      67.97
 H       2.228158     1.886156     0.860412      17.21
 C       0.328816     0.615659     0.463580      14.92
 O      -0.622708     1.248125     1.326734     180.72
 C      -0.297574     2.573704     1.982181      79.34
 H      -1.258510     2.700628     2.453809      23.63
 H       0.649666     2.477013     2.530691      23.58
 H      -0.171651     3.431396     0.986339      20.41
 C      -0.276178    -0.413944    -0.297852      -0.57
 O      -1.717478    -0.422541    -0.209531     142.48
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 C       0.503929    -1.474301    -0.885128      70.72
 H       0.183800    -2.443054    -1.529321      19.42
 C       2.435917     0.151615    -0.502799      30.14
 C       3.864156     0.624349    -0.964108      76.29
 H       3.974383     0.484943    -2.172944      20.96
 O       3.755327     2.115454    -1.144293     187.98
 H       4.292669     2.649033    -0.338541      18.46
 C       4.981969     0.233779     0.049282     102.27
 H       4.769219     0.697622     1.062785      23.72
 O       5.071527    -1.157183     0.258341     298.97
 H       4.862544    -1.551872    -0.669868      24.63
 C       6.387503     0.806716    -0.384054      78.87
 O       6.518521     2.340126    -0.364213     226.45
 H       7.178063     2.359072     0.432318      25.27
 H       6.458906     0.512190    -1.455546      31.10
 H       7.283077     0.199245     0.209538      28.97
55
name= lig-ACN-Water-frame_430
 C      -2.515069     0.958119    -3.447862      59.58
 H      -1.863160     0.045400    -3.774537      24.37
 C      -3.631209     2.191135    -1.754031      44.08
 H      -3.773011     2.333146    -0.744217      20.10
 C      -3.318611     3.468737    -2.356038       0.42
 O      -3.455156     4.724790    -1.631962     221.14
 C      -4.290773     4.887571    -0.425305     101.99
 H      -5.295875     4.606926    -0.849572      25.05
 H      -4.063770     5.749151     0.129034      26.56
 H      -4.063131     4.156419     0.229661      30.74
 C      -2.740408     3.522337    -3.647087       7.82
 O      -2.273224     4.603698    -4.318355     129.46
 H      -2.693490     5.372502    -3.932647      25.47
 C      -2.261303     2.237379    -4.040185      11.79
 H      -1.680212     2.208779    -5.122203      15.25
 C      -3.308652     0.894475    -2.347264      21.71
 C      -3.764263    -0.412411    -1.677093      68.37
 H      -4.486603    -1.119981    -2.346108      22.55
 O      -4.625235    -0.170982    -0.476309     155.48
 H      -4.095613     0.025059     0.318526      25.71
 C      -2.456415    -1.211913    -1.131022      99.42
 H      -1.954651    -1.162771    -2.098506      25.42
 C      -2.837135    -2.584174    -0.617674     116.17
 O      -3.582539    -3.356112    -1.627811     163.04
 H      -2.991477    -3.532604    -2.465423      27.53
 H      -3.571722    -2.614383     0.200022      24.93
 H      -1.887188    -3.337367    -0.421658      22.87
 C       1.916718    -1.056656    -1.035654      53.28
 H       2.610244    -1.736578    -1.549689      20.20
 C       1.634898     0.987016     0.264490      58.65
 H       2.101568     1.959430     0.769812      17.66
 C       0.273819     0.608706     0.555341       5.82
 O      -0.579155     1.284020     1.364691     212.49
 C      -0.325589     2.498119     1.983107     108.06
 H      -1.143397     2.738479     2.656953      24.77
 H       0.434294     2.493773     2.724320      25.60
 H      -0.174539     3.567718     1.245908      21.96
 C      -0.349871    -0.424136    -0.306506       7.79
 O      -1.694580    -0.383308    -0.306352     191.11
 C       0.539085    -1.399388    -0.833980      62.70
 H       0.055146    -2.448019    -1.357703      20.02
 C       2.474979     0.120598    -0.574360      22.04
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 C       3.749219     0.726092    -1.042301      87.85
 H       4.080559    -0.057021    -1.914642      19.73
 O       3.763146     2.104021    -1.170792     236.72
 H       3.984228     2.560222    -0.189139      16.80
 C       5.005871     0.311684     0.041923      86.69
 H       4.684853     0.755123     0.969497      26.01
 O       5.030359    -1.166765     0.234465     280.03
 H       5.335137    -1.521366    -0.640776      29.44
 C       6.390636     0.791644    -0.463017      99.50
 O       6.493925     2.308049    -0.348535     260.18
 H       7.000347     2.657605     0.400659      29.86
 H       6.679414     0.542832    -1.536096      32.07
 H       7.244160     0.436162     0.278081      29.70
55
name= lig-ACN-Water-frame_431
 C      -2.519649     0.984295    -3.495795      38.12
 H      -1.899301     0.072987    -3.841016      23.60
 C      -3.594975     2.172810    -1.734708      45.94
 H      -4.049521     2.020352    -0.840525      22.30
 C      -3.359947     3.468914    -2.273047       0.41
 O      -3.451498     4.709999    -1.684765     223.87
 C      -4.261270     4.813715    -0.492001     141.51
 H      -5.351027     4.809201    -0.566075      26.51
 H      -4.125969     5.799087    -0.372390      26.20
 H      -3.869308     4.244174     0.263218      28.57
 C      -2.644965     3.464230    -3.571470      -3.22
 O      -2.238011     4.611507    -4.352970     104.76
 H      -2.423609     5.539715    -3.960604      20.43
 C      -2.260946     2.228127    -4.113935      65.77
 H      -1.778561     2.246376    -5.213928      23.63
 C      -3.415142     0.872029    -2.365615      17.00
 C      -3.714123    -0.443400    -1.493974      87.41
 H      -4.282713    -1.256150    -2.243433      22.94
 O      -4.642515    -0.153741    -0.388233     174.26
 H      -4.059949     0.282333     0.360729      23.67
 C      -2.510250    -1.243746    -1.264435      96.79
 H      -1.891742    -1.652140    -2.047188      25.31
 C      -2.906984    -2.548619    -0.576987     100.31
 O      -3.638669    -3.301207    -1.672219     136.40
 H      -2.871504    -3.295897    -2.430132      26.84
 H      -3.473863    -2.236923     0.353617      24.68
 H      -1.884182    -2.967981    -0.121488      23.35
 C       1.986770    -1.160032    -0.990112      40.36
 H       2.479362    -1.811866    -1.697579      19.13
 C       1.615734     0.950212     0.283431      69.12
 H       1.838497     1.940508     0.708355      17.82
 C       0.276860     0.620126     0.490796      10.31
 O      -0.635390     1.261974     1.399303     176.37
 C      -0.315878     2.530659     2.108730      93.69
 H      -1.243251     2.844535     2.593080      23.78
 H       0.593839     2.449672     2.635680      25.09
 H      -0.060950     3.292185     1.099472      21.63
 C      -0.280150    -0.442683    -0.176053      19.86
 O      -1.735111    -0.335517    -0.301810     145.91
 C       0.564623    -1.277033    -0.857390      95.64
 H       0.063320    -2.363649    -1.309612      17.81
 C       2.398489     0.186307    -0.605025      28.51
 C       3.853174     0.631396    -0.941233      83.09
 H       4.128008     0.574426    -2.148795      22.20
 O       3.732002     2.156651    -1.232607     154.28
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 H       3.994034     2.673845    -0.361022      21.57
 C       4.962193     0.321905    -0.048179     101.26
 H       4.867986     0.721929     0.895994      28.18
 O       5.017919    -1.098155     0.228599     332.87
 H       5.203810    -1.517292    -0.610158      33.38
 C       6.390852     0.887263    -0.459675      88.46
 O       6.485179     2.260774    -0.388398     314.17
 H       7.041552     2.334314     0.388787      27.17
 H       6.570506     0.494902    -1.520588      32.35
 H       7.068448     0.278724     0.233726      31.53
55
name= lig-ACN-Water-frame_432
 C      -2.582046     0.957661    -3.544317      54.66
 H      -2.595694     0.048918    -4.178946      21.08
 C      -3.713386     2.160301    -1.671624      68.87
 H      -4.431996     2.302173    -0.933372      20.32
 C      -3.256829     3.380159    -2.324509       5.09
 O      -3.486139     4.655519    -1.770021     203.46
 C      -4.238674     4.849443    -0.506261     133.75
 H      -5.150460     4.386219    -0.719136      26.58
 H      -4.288605     5.797213    -0.201037      27.45
 H      -3.856773     4.290039     0.336293      27.24
 C      -2.535654     3.453142    -3.531472       0.39
 O      -2.245528     4.540688    -4.325204     194.53
 H      -2.400500     5.472374    -3.816476      16.93
 C      -2.270313     2.192506    -4.185122      30.54
 H      -1.504132     2.260366    -5.039394      25.83
 C      -3.359369     0.983819    -2.312782      25.87
 C      -3.787333    -0.308237    -1.543328      64.38
 H      -4.672150    -0.884294    -2.223055      23.44
 O      -4.580688    -0.142277    -0.328984     154.03
 H      -4.037512     0.150289     0.490310      23.59
 C      -2.421289    -1.215029    -1.214791      85.93
 H      -1.961455    -1.187804    -2.176853      26.29
 C      -2.958781    -2.545159    -0.551222     112.06
 O      -3.645562    -3.241748    -1.611200     173.58
 H      -2.996545    -3.655224    -2.218505      30.88
 H      -3.914914    -2.487995     0.130347      23.56
 H      -2.247932    -3.362547    -0.183602      25.51
 C       1.921528    -1.051186    -0.986422      35.60
 H       2.568605    -1.720360    -1.519379      22.96
 C       1.605237     0.989925     0.295170      65.94
 H       2.209988     1.744748     0.642785      21.45
 C       0.213034     0.694510     0.567355      14.17
 O      -0.683606     1.238841     1.456000     207.21
 C      -0.244882     2.527596     2.090288     106.51
 H      -1.124360     2.760556     2.728379      24.00
 H       0.470046     2.405467     2.797542      27.59
 H      -0.042137     3.513453     1.360344      23.18
 C      -0.348516    -0.461538    -0.148410       7.05
 O      -1.700960    -0.396638    -0.300185     170.35
 C       0.558898    -1.358155    -0.910725      74.89
 H       0.099604    -2.276064    -1.643681      18.82
 C       2.490053     0.133639    -0.567056      26.29
 C       3.820750     0.738530    -1.029825      68.98
 H       4.021799    -0.042697    -1.972363      23.64
 O       3.719206     2.213001    -1.221821     151.58
 H       4.044071     2.597544    -0.399537      24.96
 C       4.993490     0.347133     0.025629     109.92
 H       4.707632     0.809691     0.851538      29.56
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 O       5.026196    -1.056790     0.220104     327.82
 H       4.880751    -1.490545    -0.657732      29.69
 C       6.334552     0.768771    -0.498622     104.68
 O       6.542237     2.300959    -0.415329     270.96
 H       7.177383     2.559957     0.321614      25.96
 H       6.540163     0.522993    -1.592822      31.53
 H       7.134062     0.364356     0.091796      31.06
55
name= lig-ACN-Water-frame_433
 C      -2.787620     0.963509    -3.549038      54.36
 H      -2.757243     0.015406    -4.039338      26.15
 C      -3.778781     2.303779    -1.742436      58.79
 H      -4.336144     2.253344    -0.779945      21.14
 C      -3.189842     3.396491    -2.282553      18.47
 O      -3.518211     4.671384    -1.831703     206.71
 C      -4.247648     4.771611    -0.552719     128.15
 H      -5.176407     4.353378    -0.553521      29.56
 H      -4.403919     5.774169    -0.553978      26.76
 H      -3.483786     4.425231     0.217507      26.21
 C      -2.464925     3.339351    -3.568122       5.01
 O      -2.224191     4.483763    -4.262926     149.19
 H      -2.748571     5.340424    -3.884294      21.18
 C      -2.211190     2.108521    -4.171291      69.55
 H      -1.817499     2.059424    -5.172422      22.50
 C      -3.299208     1.025674    -2.236886      24.45
 C      -3.806199    -0.220889    -1.589797      82.34
 H      -4.410274    -0.971092    -2.405294      23.17
 O      -4.513382    -0.079666    -0.281380     170.27
 H      -3.819220    -0.147315     0.367361      27.70
 C      -2.521212    -1.177036    -1.158534      91.03
 H      -1.902448    -1.497326    -1.958817      26.52
 C      -3.004717    -2.569542    -0.594195     116.51
 O      -3.702826    -3.273786    -1.631870     224.38
 H      -3.008203    -3.703058    -2.093392      31.21
 H      -3.606751    -2.124472     0.333641      25.27
 H      -2.156262    -3.005721    -0.038881      26.74
 C       1.876738    -0.984065    -1.070972      57.37
 H       2.487524    -1.653999    -1.646148      22.76
 C       1.608283     1.019621     0.338450      79.01
 H       1.756115     1.822744     0.929319      21.40
 C       0.270364     0.589966     0.568001      -9.57
 O      -0.661028     1.321600     1.503319     177.82
 C      -0.243478     2.479664     2.152896      99.79
 H      -1.083862     2.977490     2.725368      23.94
 H       0.626643     2.300623     2.642608      27.57
 H       0.098232     3.224669     1.254577      23.47
 C      -0.283143    -0.462181    -0.261797      18.78
 O      -1.685592    -0.460226    -0.224926     190.28
 C       0.476472    -1.352673    -0.884673      58.03
 H       0.047832    -2.237269    -1.572968      20.48
 C       2.423930     0.201255    -0.432285      29.85
 C       3.761166     0.772415    -0.993649      77.14
 H       4.123007     0.587634    -2.175118      21.79
 O       3.738574     2.193287    -1.194993     217.32
 H       3.857789     2.660376    -0.385148      26.52
 C       4.943474     0.424944     0.036405     108.64
 H       4.862788     0.750171     0.941697      28.67
 O       5.002659    -1.071092     0.231099     275.64
 H       5.244198    -1.491005    -0.713990      26.61
 C       6.405057     0.821240    -0.523411      96.49
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 O       6.601070     2.287231    -0.481429     275.30
 H       7.177482     2.292222     0.402381      23.53
 H       6.329561     0.455669    -1.582471      31.21
 H       7.107518     0.251992    -0.027225      32.12
55
name= lig-ACN-Water-frame_434
 C      -2.865305     0.918668    -3.523379      50.82
 H      -2.685291    -0.099547    -3.820904      24.33
 C      -3.682797     2.306388    -1.729731      57.90
 H      -4.196646     2.374038    -0.683793      19.20
 C      -3.172798     3.496084    -2.333760      22.05
 O      -3.550537     4.741886    -1.913872     247.57
 C      -4.216684     4.757182    -0.630107     134.78
 H      -4.982514     4.156091    -0.554962      30.41
 H      -4.543259     5.760274    -0.426065      26.33
 H      -3.589072     4.481430     0.342615      26.12
 C      -2.483264     3.309606    -3.530185      -2.25
 O      -2.159334     4.443061    -4.252524     172.06
 H      -2.513328     5.352445    -3.889791      22.11
 C      -2.254038     1.980666    -4.167609      52.36
 H      -2.096276     1.960854    -5.166845      24.36
 C      -3.442249     1.057236    -2.225793      37.05
 C      -3.674174    -0.286843    -1.466937      94.27
 H      -4.540483    -0.852742    -2.200106      21.87
 O      -4.470209    -0.006266    -0.317301     216.52
 H      -3.989230     0.191734     0.517439      22.71
 C      -2.588299    -1.219665    -1.250726      77.10
 H      -2.027247    -1.347912    -2.149552      24.42
 C      -3.018457    -2.451359    -0.539828     112.47
 O      -3.751864    -3.349188    -1.614300      91.81
 H      -3.054320    -3.517663    -2.394832      28.06
 H      -3.848454    -2.689283     0.256369      22.32
 H      -2.175630    -3.039716    -0.410826      25.07
 C       1.857609    -0.933216    -1.096393      25.61
 H       2.480521    -1.396053    -1.858035      19.85
 C       1.518465     1.008751     0.507169      85.33
 H       2.026418     1.909430     0.754105      18.01
 C       0.227006     0.596333     0.629085      23.10
 O      -0.624502     1.231108     1.416884     186.07
 C      -0.123314     2.505772     2.162528      94.78
 H      -1.042164     2.773703     2.773322      24.03
 H       0.579882     2.380472     2.853212      27.27
 H       0.062867     3.366814     1.385458      22.54
 C      -0.368624    -0.369483    -0.216668       2.58
 O      -1.733641    -0.504565    -0.092818     109.27
 C       0.552759    -1.322849    -0.969335      67.31
 H       0.124848    -2.283852    -1.333105      16.17
 C       2.360478     0.261161    -0.504134      32.00
 C       3.780567     0.781499    -0.822786      74.10
 H       3.857184     0.103472    -1.866757      22.05
 O       3.731643     2.255388    -1.130588     204.10
 H       3.762464     2.680268    -0.189973      25.20
 C       4.985391     0.370247    -0.015233     106.86
 H       4.773026     0.821746     0.806824      31.14
 O       4.979383    -1.037718     0.213212     328.41
 H       5.414531    -1.492916    -0.592784      29.55
 C       6.334351     0.867115    -0.577009     120.35
 O       6.699444     2.220827    -0.527938     313.56
 H       7.214635     2.534567     0.323649      27.48
 H       6.540162     0.631244    -1.636296      31.04
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 H       7.028871     0.355030    -0.049181      31.58
55
name= lig-ACN-Water-frame_435
 C      -2.822069     0.801598    -3.447020      66.10
 H      -2.818412    -0.117088    -4.091244      22.25
 C      -3.556964     2.310640    -1.602336      52.72
 H      -4.117277     2.451278    -0.580850      17.34
 C      -3.245925     3.430962    -2.375121      -3.95
 O      -3.561176     4.828328    -1.965293     239.89
 C      -4.223713     4.815290    -0.638516     108.65
 H      -4.950855     4.174429    -0.769858      29.02
 H      -4.756917     5.798192    -0.451475      24.51
 H      -3.356403     4.425915     0.066301      24.02
 C      -2.501526     3.320977    -3.618659      16.91
 O      -2.036148     4.404180    -4.316061     217.01
 H      -2.377122     5.161321    -3.837703      22.20
 C      -2.438291     2.052683    -4.152363      59.46
 H      -1.792563     1.959530    -4.912955      26.71
 C      -3.497899     0.978455    -2.271756      22.41
 C      -3.779473    -0.199987    -1.422024      90.68
 H      -4.464594    -1.046466    -2.078272      21.54
 O      -4.512263     0.051433    -0.256630     223.51
 H      -3.850033     0.477419     0.426274      21.97
 C      -2.513979    -1.160544    -1.139650      74.95
 H      -1.876428    -1.318539    -2.012900      23.90
 C      -3.032703    -2.643146    -0.654738     113.77
 O      -3.748476    -3.386509    -1.566556     219.98
 H      -3.192506    -3.346861    -2.460015      27.58
 H      -3.593697    -2.151530     0.271932      23.41
 H      -2.236293    -3.072445    -0.173432      28.14
 C       1.895598    -0.808149    -1.142212      69.40
 H       2.568899    -1.436412    -1.755930      15.12
 C       1.625354     0.908345     0.477337      67.13
 H       1.895240     1.812394     1.130873      13.22
 C       0.198669     0.628841     0.593469       9.36
 O      -0.665415     1.288687     1.491346     205.54
 C      -0.131073     2.450370     2.150878     106.61
 H      -1.041446     2.787190     2.740674      22.52
 H       0.713020     2.164624     2.612529      27.58
 H       0.167929     3.235818     1.421005      25.53
 C      -0.372482    -0.467102    -0.189630      13.87
 O      -1.796965    -0.603060    -0.058394     201.36
 C       0.467370    -1.188504    -0.959135      79.50
 H       0.208076    -2.029747    -1.476660      22.20
 C       2.328719     0.315668    -0.452435      41.83
 C       3.688215     0.787592    -0.840163      69.94
 H       4.059994     0.444557    -1.980707      22.12
 O       3.735541     2.262682    -1.034019     167.08
 H       4.044159     2.816043    -0.153301      22.11
 C       4.978170     0.407825     0.045008      95.47
 H       5.084766     0.691666     0.960521      29.11
 O       4.999454    -1.036154     0.196765     341.42
 H       5.050212    -1.448287    -0.655443      29.63
 C       6.360023     0.779142    -0.649984     101.10
 O       6.747180     2.274975    -0.582281     230.95
 H       7.287086     2.301586     0.282001      25.04
 H       6.271309     0.426101    -1.667447      33.38
 H       7.042950     0.236809    -0.138098      33.40
55
name= lig-ACN-Water-frame_436
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 C      -2.826555     0.899755    -3.495466      75.42
 H      -2.711447    -0.175391    -3.944321      22.63
 C      -3.499121     2.254694    -1.627604      48.87
 H      -3.881868     2.220913    -0.563947      18.51
 C      -3.295732     3.502941    -2.382178      29.68
 O      -3.547093     4.779877    -1.991015     253.60
 C      -4.243429     4.848358    -0.709885     127.53
 H      -5.059529     4.294936    -0.507694      28.01
 H      -4.375289     6.002119    -0.631563      24.38
 H      -3.607191     4.660566     0.278573      23.99
 C      -2.644658     3.335199    -3.633633       5.08
 O      -1.926165     4.386905    -4.356747     124.18
 H      -2.385633     5.207890    -4.296477      25.86
 C      -2.453254     1.995575    -4.184742      65.43
 H      -1.909302     1.922341    -5.066840      27.10
 C      -3.427162     0.999755    -2.162465      31.08
 C      -3.876271    -0.284114    -1.414497      70.11
 H      -4.682562    -0.944170    -2.120307      21.54
 O      -4.608151     0.122608    -0.150245     156.88
 H      -3.945981     0.241285     0.669723      20.03
 C      -2.529615    -1.216596    -1.088534      65.73
 H      -1.908380    -1.135299    -2.026083      22.00
 C      -2.948028    -2.621324    -0.611585     105.52
 O      -3.744105    -3.433751    -1.603714     197.20
 H      -3.201530    -3.659472    -2.342726      31.60
 H      -3.876405    -2.602191     0.121757      22.36
 H      -2.239356    -3.253812    -0.279597      26.78
 C       1.786985    -0.766139    -1.169867      25.40
 H       2.366067    -1.375986    -1.923219      24.34
 C       1.506869     0.940200     0.546512      72.28
 H       2.086957     1.643973     1.279672      18.43
 C       0.180862     0.617020     0.593462      20.60
 O      -0.724617     1.295825     1.513373     214.17
 C      -0.142126     2.420501     2.175114     117.09
 H      -0.731758     2.967534     2.899931      24.42
 H       0.673387     2.232913     2.763315      26.55
 H       0.109464     3.151953     1.305343      23.42
 C      -0.399721    -0.452702    -0.088831      13.39
 O      -1.732055    -0.678843     0.016963     172.62
 C       0.478813    -1.152921    -1.047675      42.99
 H       0.094307    -1.779926    -1.645421      21.32
 C       2.462101     0.267758    -0.457703      22.86
 C       3.823525     0.921244    -0.846239      80.96
 H       3.903525     0.459949    -2.014281      21.01
 O       3.734356     2.290525    -0.967576     235.35
 H       3.806932     2.721339     0.058170      20.86
 C       4.997338     0.418477     0.072279     106.43
 H       4.794688     0.862381     0.909154      29.20
 O       5.015724    -1.076105     0.168013     315.63
 H       4.798144    -1.380889    -0.738781      29.39
 C       6.357290     0.766618    -0.687577     108.28
 O       6.733207     2.204349    -0.665197     243.94
 H       7.136160     2.445997     0.214200      27.81
 H       6.307765     0.628746    -1.730149      33.90
 H       7.163288     0.160090    -0.375904      32.88
55
name= lig-ACN-Water-frame_437
 C      -2.892598     0.889104    -3.447632      49.73
 H      -2.633832    -0.153976    -3.926795      24.78
 C      -3.543613     2.327327    -1.636078      61.88
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 H      -3.798723     2.580454    -0.633882      22.82
 C      -3.261790     3.410643    -2.422163      11.81
 O      -3.563962     4.688577    -1.931207     220.50
 C      -4.244696     4.988012    -0.701578     109.69
 H      -5.178898     4.577468    -0.852876      28.06
 H      -4.511504     6.181428    -0.676637      24.49
 H      -3.531731     4.552216     0.082817      25.83
 C      -2.665877     3.344301    -3.752781       7.18
 O      -1.932473     4.332176    -4.354260     164.95
 H      -2.443801     5.217133    -4.205967      23.61
 C      -2.396499     2.085299    -4.231361      42.71
 H      -2.255029     1.961371    -5.311530      19.81
 C      -3.302842     0.969461    -2.147885      25.32
 C      -3.823774    -0.272096    -1.257027      90.17
 H      -4.670206    -0.869899    -1.923649      23.11
 O      -4.671567     0.143651    -0.136965     174.43
 H      -4.066043     0.157529     0.660815      24.55
 C      -2.684102    -1.281453    -1.079353      58.54
 H      -2.120506    -1.479048    -2.083674      23.03
 C      -2.977499    -2.702329    -0.576178     115.87
 O      -3.693822    -3.450623    -1.676664     201.20
 H      -2.916021    -3.791831    -2.143702      29.39
 H      -3.406621    -2.651188     0.482716      25.35
 H      -2.025719    -3.011502    -0.450497      26.55
 C       1.835161    -0.736054    -1.223459      75.19
 H       2.361446    -1.049323    -2.166554      13.54
 C       1.578466     0.925651     0.516881      61.79
 H       1.951630     1.804083     1.124623      18.66
 C       0.146882     0.622926     0.739051       0.34
 O      -0.757205     1.227541     1.516437     172.61
 C      -0.132325     2.511644     2.210434      87.27
 H      -1.057524     2.718821     2.661308      24.33
 H       0.828839     2.156186     2.698952      23.91
 H       0.167775     3.238539     1.444148      26.43
 C      -0.360279    -0.441586    -0.147987       3.16
 O      -1.728856    -0.731761     0.134172     101.35
 C       0.382631    -1.113439    -1.079468      79.46
 H       0.040646    -1.833668    -1.597763      26.04
 C       2.377501     0.276805    -0.392262      36.19
 C       3.850325     0.856514    -0.815313      49.07
 H       4.206897     0.536419    -1.999579      21.41
 O       3.731397     2.389276    -0.905206     203.55
 H       3.666514     2.828556     0.088741      21.22
 C       5.062030     0.373835    -0.025499     114.46
 H       5.118463     0.641407     0.921440      29.08
 O       4.996897    -1.048306     0.139752     283.86
 H       5.007673    -1.528094    -0.805041      29.05
 C       6.346321     0.782468    -0.720705     104.63
 O       6.712228     2.131721    -0.716848     293.66
 H       7.112032     2.318815     0.193981      28.34
 H       6.120887     0.454329    -1.680090      36.03
 H       7.148727     0.182115    -0.289883      31.74
55
name= lig-ACN-Water-frame_438
 C      -2.805707     0.890115    -3.459569      63.38
 H      -2.906415    -0.104268    -4.018970      19.91
 C      -3.572509     2.288254    -1.629465      63.93
 H      -4.051985     2.389357    -0.735006      23.13
 C      -3.243752     3.418091    -2.455546      17.39
 O      -3.511511     4.710357    -1.967237     184.96
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 C      -4.286447     5.037460    -0.721459     113.16
 H      -5.329314     4.720115    -0.608407      25.52
 H      -4.083677     6.236686    -0.713668      23.80
 H      -3.975138     4.729020     0.330821      24.13
 C      -2.591548     3.302136    -3.719643      13.97
 O      -2.022227     4.401118    -4.377485     126.00
 H      -2.357818     5.323572    -3.933573      18.34
 C      -2.541402     1.963798    -4.253743      48.63
 H      -1.909742     1.854829    -5.225674      27.09
 C      -3.305651     1.008607    -2.045079      25.91
 C      -3.771755    -0.176512    -1.225901      95.62
 H      -4.448849    -0.785746    -2.055080      22.68
 O      -4.629386     0.161542    -0.135050     223.77
 H      -4.161416     0.434154     0.643486      24.95
 C      -2.749168    -1.288251    -0.885138      75.38
 H      -2.125780    -1.203852    -1.901840      22.83
 C      -2.955856    -2.807296    -0.584094     120.77
 O      -3.624483    -3.452304    -1.617751     227.44
 H      -3.038980    -3.625152    -2.517912      25.26
 H      -3.603506    -3.025510     0.297783      24.56
 H      -2.051897    -3.309583    -0.452390      25.86
 C       1.785310    -0.694172    -1.275440      39.10
 H       2.465921    -1.253589    -1.964327      25.85
 C       1.554937     0.956855     0.564511      69.42
 H       1.919991     1.848560     0.976063      18.49
 C       0.253539     0.509725     0.685826       6.14
 O      -0.685320     1.283429     1.582417     198.45
 C      -0.276505     2.463678     2.189188     121.65
 H      -0.855506     2.969856     2.903565      25.59
 H       0.587030     2.273528     3.001170      24.27
 H       0.009069     3.161526     1.485979      27.92
 C      -0.423510    -0.423673    -0.133176      -2.06
 O      -1.774431    -0.811325     0.121810     150.50
 C       0.468340    -1.069130    -1.112390      48.34
 H       0.098414    -1.836935    -1.673815      21.65
 C       2.369839     0.300164    -0.461406      25.70
 C       3.699913     0.897715    -0.747526      73.09
 H       3.746917     0.632985    -1.985522      19.76
 O       3.723102     2.367791    -0.848280     216.39
 H       4.042846     2.744282     0.027865      23.41
 C       5.072823     0.353199     0.002420      98.29
 H       5.153425     0.816995     0.900531      26.62
 O       4.985408    -1.090974     0.074333     338.17
 H       5.213094    -1.447766    -0.845854      27.95
 C       6.379493     0.644282    -0.828703     104.89
 O       6.725631     2.133750    -0.732051     224.78
 H       7.221839     2.242952     0.189183      26.51
 H       6.516572     0.438847    -1.829186      33.54
 H       7.182613     0.037150    -0.277754      31.04
55
name= lig-ACN-Water-frame_439
 C      -2.806603     0.783758    -3.340736      57.55
 H      -2.721593    -0.257721    -3.678862      22.81
 C      -3.595128     2.321644    -1.631148      72.44
 H      -4.198625     2.430254    -0.804712      22.46
 C      -3.275770     3.462298    -2.365645       7.49
 O      -3.460431     4.788861    -1.987293     181.89
 C      -4.292419     5.064430    -0.752929     105.88
 H      -5.347186     4.948023    -1.102007      24.48
 H      -4.206887     6.296515    -0.625940      23.40
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 H      -3.742951     4.462391    -0.043944      23.43
 C      -2.554297     3.274768    -3.625182       0.23
 O      -2.122512     4.417821    -4.385398     145.37
 H      -2.718106     5.358517    -4.227470      15.51
 C      -2.553194     1.956579    -4.233995      34.43
 H      -2.055007     1.668034    -5.302595      25.59
 C      -3.270656     1.017535    -2.116867      42.94
 C      -3.791142    -0.217360    -1.239783      81.19
 H      -4.621110    -0.784722    -1.896399      24.78
 O      -4.585681     0.240193    -0.117815     184.76
 H      -4.045455     0.068842     0.696262      24.13
 C      -2.576833    -1.272268    -0.825501      74.86
 H      -2.004347    -1.485964    -1.862423      23.07
 C      -2.960069    -2.846908    -0.513971     101.93
 O      -3.653069    -3.517897    -1.651528     187.49
 H      -3.087646    -3.248621    -2.512622      26.92
 H      -3.612976    -2.967973     0.328587      25.21
 H      -1.986252    -3.199792    -0.220517      26.65
 C       1.800401    -0.663886    -1.251354      66.17
 H       2.360425    -1.343343    -1.910310      22.13
 C       1.514368     0.949932     0.527023      60.17
 H       1.909870     1.658861     1.130093      19.87
 C       0.132276     0.588387     0.734355       9.76
 O      -0.652311     1.182132     1.594696     222.13
 C      -0.314558     2.504921     2.235870      94.77
 H      -1.309250     2.627294     2.549267      23.36
 H       0.722511     2.452825     2.876955      21.68
 H      -0.096050     3.199254     1.542096      28.08
 C      -0.423775    -0.500870    -0.146643      14.51
 O      -1.730598    -0.814316     0.175784     212.48
 C       0.406525    -1.081526    -1.093368      51.50
 H       0.065104    -1.861858    -1.792932      20.26
 C       2.340636     0.386416    -0.460579      37.15
 C       3.709954     0.940923    -0.797691      81.69
 H       4.020654     0.529932    -1.938914      21.29
 O       3.709528     2.340289    -0.780804     249.63
 H       3.760348     2.689160     0.118846      23.51
 C       5.006214     0.317631    -0.119477     100.02
 H       5.057464     0.639951     0.872777      23.96
 O       4.978884    -1.156365     0.025757     358.29
 H       5.013352    -1.502180    -0.851082      29.40
 C       6.448388     0.655318    -0.845384      86.08
 O       6.777624     2.046213    -0.747999     305.18
 H       7.089219     2.237501     0.233376      26.54
 H       6.224675     0.344822    -1.831327      32.96
 H       7.296464    -0.023311    -0.390357      30.05
55
name= lig-ACN-Water-frame_440
 C      -2.762949     0.785683    -3.382282      49.52
 H      -2.428915    -0.132611    -3.748653      24.37
 C      -3.657746     2.349991    -1.601624      50.00
 H      -4.116044     2.423850    -0.604343      19.55
 C      -3.206287     3.499926    -2.352938      19.97
 O      -3.431579     4.889745    -2.001555     235.41
 C      -4.247093     5.072028    -0.887235     124.08
 H      -5.372600     4.720993    -0.996943      25.96
 H      -4.110875     6.126571    -0.374777      25.58
 H      -4.169796     4.427739    -0.013759      26.56
 C      -2.630031     3.281099    -3.623048       9.89
 O      -2.217212     4.277859    -4.400872     125.61
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 H      -2.621926     5.283966    -4.095563      19.60
 C      -2.424106     1.949635    -4.054202      45.13
 H      -2.339540     2.026758    -5.255918      21.06
 C      -3.362895     0.970421    -2.010197      12.64
 C      -3.747322    -0.294177    -1.224516      87.40
 H      -4.409769    -1.023182    -1.882752      24.67
 O      -4.519027     0.281511    -0.075943     180.85
 H      -4.092833     0.143021     0.881113      20.03
 C      -2.562962    -1.374390    -0.957206      48.54
 H      -1.782461    -1.377331    -1.836906      20.78
 C      -3.006019    -2.772465    -0.463196     113.88
 O      -3.681586    -3.513661    -1.602903     223.31
 H      -3.027328    -3.676560    -2.308642      28.86
 H      -3.608196    -2.684973     0.354344      27.19
 H      -2.168346    -3.491404    -0.289538      24.01
 C       1.742079    -0.694821    -1.201051      26.94
 H       2.364009    -0.969620    -2.045798      15.76
 C       1.463970     0.992676     0.520204      61.88
 H       1.769369     1.691019     1.257749      16.54
 C       0.139865     0.591487     0.627571      15.51
 O      -0.718096     1.096792     1.678428     200.82
 C      -0.396224     2.510575     2.190820     106.98
 H      -1.166954     2.826467     2.892650      23.75
 H       0.356055     2.335785     3.165579      21.15
 H      -0.217074     3.204831     1.547813      28.50
 C      -0.349096    -0.466744    -0.065947      17.48
 O      -1.686551    -0.786201     0.272463     122.28
 C       0.414442    -1.101821    -1.073629      92.82
 H      -0.030492    -2.034512    -1.663059      20.17
 C       2.298070     0.366761    -0.495090      40.73
 C       3.815796     0.852799    -0.921916      61.30
 H       3.782719     0.917521    -2.093748      22.02
 O       3.711370     2.405130    -0.711278     187.42
 H       3.818626     2.652152     0.188163      24.43
 C       5.057779     0.228297    -0.156109      89.07
 H       4.989809     0.608026     0.867556      23.97
 O       4.941064    -1.200121    -0.048954     325.88
 H       4.832785    -1.668913    -0.895457      30.87
 C       6.324095     0.648995    -0.829929      96.39
 O       6.856866     1.978232    -0.771645     265.12
 H       7.139400     2.120639     0.201363      28.79
 H       6.377635     0.563606    -1.909905      29.98
 H       7.150152    -0.161176    -0.452784      28.45
55
name= lig-ACN-Water-frame_441
 C      -2.754437     0.861731    -3.249864      59.79
 H      -2.709526    -0.047380    -3.750339      25.53
 C      -3.645812     2.288470    -1.571673      60.71
 H      -4.060890     2.470042    -0.504749      21.60
 C      -3.225662     3.503069    -2.261844      23.88
 O      -3.369027     4.870984    -2.033334     213.39
 C      -4.322209     5.044919    -0.850560     103.05
 H      -5.359060     5.086481    -1.363581      26.34
 H      -4.163835     6.169778    -0.698481      26.41
 H      -3.885647     4.443034    -0.098516      26.56
 C      -2.700115     3.241609    -3.580900      10.27
 O      -2.266310     4.177483    -4.496988     127.64
 H      -2.434466     5.184356    -4.182280      21.95
 C      -2.354756     1.982874    -4.015193      49.45
 H      -1.676616     1.758429    -4.973184      22.04
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 C      -3.384959     0.970341    -2.066643      43.40
 C      -3.690653    -0.304597    -1.160230      94.95
 H      -4.550142    -0.801183    -1.706522      24.68
 O      -4.456022     0.188521    -0.032740     192.99
 H      -3.765736     0.489035     0.672057      24.25
 C      -2.532756    -1.308567    -0.888723      82.03
 H      -2.037848    -1.386086    -1.923794      24.28
 C      -3.034468    -2.752147    -0.526694     118.02
 O      -3.737401    -3.468874    -1.482815     241.88
 H      -3.157342    -3.964504    -2.019744      30.32
 H      -3.766260    -2.590123     0.156794      27.69
 H      -2.136134    -3.162845     0.095137      26.15
 C       1.745769    -0.701456    -1.272813      42.02
 H       2.213605    -1.290425    -2.060664      24.40
 C       1.533036     1.062737     0.491468      61.07
 H       2.074195     1.993562     0.939672      18.62
 C       0.155985     0.662402     0.720838      -8.07
 O      -0.767357     1.103388     1.731841     204.46
 C      -0.507272     2.384765     2.228702     112.55
 H      -1.444988     2.827669     2.600127      24.09
 H       0.625923     2.443704     2.704680      22.15
 H      -0.296821     2.900240     1.466032      30.42
 C      -0.422777    -0.497145    -0.050752      -4.79
 O      -1.713675    -0.840145     0.228920     161.35
 C       0.425236    -1.145459    -0.985016      44.86
 H       0.050592    -2.183936    -1.609870      18.66
 C       2.357555     0.369974    -0.510775      25.40
 C       3.663000     0.954177    -0.904990     100.45
 H       3.938344     0.613222    -1.946101      23.34
 O       3.767174     2.379951    -0.681245     201.17
 H       3.977483     2.516256     0.248671      25.36
 C       4.957171     0.204612    -0.189790      91.50
 H       5.060289     0.603202     0.865838      24.44
 O       4.894671    -1.266663    -0.123179     293.47
 H       4.954081    -1.508393    -1.133176      26.83
 C       6.351262     0.560673    -0.939881      80.80
 O       6.896594     1.954500    -0.738655     217.55
 H       7.338136     2.037923     0.167146      25.48
 H       6.093805     0.268422    -1.997081      30.91
 H       7.149797    -0.213198    -0.453114      29.92
55
name= lig-ACN-Water-frame_442
 C      -2.734000     0.811256    -3.263711      70.01
 H      -2.610868    -0.221326    -3.551924      23.64
 C      -3.584524     2.325890    -1.476255      61.88
 H      -4.217022     2.326322    -0.483522      18.69
 C      -3.283467     3.403720    -2.321575       8.86
 O      -3.383743     4.758589    -1.945574     236.64
 C      -4.311027     5.158841    -0.911626     136.95
 H      -5.406292     4.675106    -1.076091      24.85
 H      -4.240391     6.171698    -0.560371      27.06
 H      -4.313844     4.533446    -0.039233      26.27
 C      -2.629091     3.223666    -3.605043      13.58
 O      -2.302035     4.174435    -4.583423     182.68
 H      -2.698003     5.093512    -4.377272      20.41
 C      -2.315068     1.908847    -3.996206      45.23
 H      -1.573861     1.850400    -4.859272      28.83
 C      -3.394153     1.022768    -1.966290      21.19
 C      -3.760930    -0.198324    -1.190036     103.06
 H      -4.348546    -0.935445    -1.774089      26.98
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 O      -4.395859     0.055364     0.055854     205.47
 H      -3.860075     0.350869     0.798754      24.67
 C      -2.569672    -1.231970    -0.913466      83.14
 H      -1.867084    -1.352459    -1.751672      26.33
 C      -3.101814    -2.619669    -0.385579      99.61
 O      -3.796619    -3.492608    -1.427926     155.96
 H      -3.090764    -3.681524    -2.211005      26.20
 H      -3.731923    -2.517125     0.438499      27.26
 H      -2.212386    -3.369035    -0.131976      24.18
 C       1.744760    -0.715713    -1.260632      58.82
 H       2.470036    -1.264333    -1.863326      23.67
 C       1.479559     1.050817     0.433546      67.46
 H       1.875344     2.103881     0.971266      20.08
 C       0.164000     0.582214     0.795254      20.11
 O      -0.755872     1.025768     1.700686     201.62
 C      -0.538405     2.417182     2.162072     116.23
 H      -1.424226     2.541273     2.869273      25.63
 H       0.240179     2.481371     3.068162      24.12
 H      -0.526040     3.051417     1.490227      31.84
 C      -0.352776    -0.429095    -0.007883       5.90
 O      -1.739443    -0.887389     0.187347     160.76
 C       0.456753    -1.150403    -0.881496      47.60
 H      -0.090003    -2.160091    -1.526134      19.97
 C       2.236597     0.376538    -0.549199      24.11
 C       3.695521     0.926962    -0.850049     104.78
 H       3.664720     0.960779    -1.962480      24.10
 O       3.828496     2.337990    -0.694666     192.89
 H       3.840428     2.755673     0.264618      22.55
 C       4.905442     0.213102    -0.232704      91.06
 H       4.920154     0.385287     0.908058      25.55
 O       4.829482    -1.248707    -0.202769     290.85
 H       4.796690    -1.713301    -1.156884      26.15
 C       6.345006     0.521495    -0.960441      85.89
 O       6.866878     1.837533    -0.782166     216.05
 H       7.035831     1.872511     0.197555      28.11
 H       6.356474     0.526584    -2.119310      28.00
 H       7.160285    -0.327331    -0.644592      30.32
55
name= lig-ACN-Water-frame_443
 C      -2.741195     0.753656    -3.197295      60.47
 H      -2.348036    -0.232245    -3.551103      24.89
 C      -3.573691     2.327499    -1.461674      50.36
 H      -4.050672     2.689835    -0.482659      20.30
 C      -3.286984     3.421128    -2.383166       3.85
 O      -3.408600     4.683130    -1.863139     215.02
 C      -4.388942     5.122913    -0.879714     118.49
 H      -5.452596     5.101281    -1.392167      23.94
 H      -4.231801     6.153535    -1.050798      25.66
 H      -4.000178     4.912144     0.118791      25.90
 C      -2.571378     3.181573    -3.644726       3.22
 O      -2.363053     4.200725    -4.585178     185.90
 H      -2.522473     5.104795    -4.272407      25.82
 C      -2.274098     1.820793    -4.002387      43.52
 H      -2.107977     1.660089    -5.050123      22.96
 C      -3.326908     1.034635    -1.935585      40.47
 C      -3.752350    -0.237883    -1.172888      88.83
 H      -4.603455    -0.539580    -1.776126      24.52
 O      -4.450244    -0.059048     0.141704     152.30
 H      -3.813401    -0.206100     0.842884      26.58
 C      -2.612972    -1.258343    -0.960759      63.09
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 H      -2.142144    -1.443558    -1.889044      26.50
 C      -3.158509    -2.595201    -0.361006      96.24
 O      -3.826985    -3.456957    -1.373996     155.04
 H      -3.305731    -3.242836    -2.245959      28.46
 H      -3.836290    -2.513854     0.513534      24.40
 H      -2.110926    -3.066042     0.028677      23.75
 C       1.760914    -0.757534    -1.135771      45.69
 H       2.272922    -1.281429    -1.958949      19.68
 C       1.333657     1.050896     0.456466      62.34
 H       1.757017     1.999615     1.176546      19.44
 C       0.149385     0.489434     0.762469      28.08
 O      -0.711525     1.036693     1.698651     238.25
 C      -0.645143     2.438093     2.220473     100.45
 H      -1.588902     2.637652     2.820053      25.12
 H       0.406422     2.493640     2.645528      24.15
 H      -0.592426     3.078898     1.549102      32.16
 C      -0.386606    -0.528830    -0.010346      14.77
 O      -1.657793    -0.809878     0.249768     101.75
 C       0.479962    -1.180628    -0.904839      55.91
 H      -0.047881    -2.290773    -1.440875      18.84
 C       2.232153     0.451622    -0.545142       4.92
 C       3.690894     0.886368    -0.915540      91.86
 H       3.880720     0.615946    -1.988887      24.74
 O       3.863745     2.398683    -0.704453     170.08
 H       3.924168     2.463481     0.388407      21.87
 C       4.971247     0.131628    -0.290651      83.39
 H       5.113344     0.664159     0.704076      25.55
 O       4.724919    -1.239193    -0.257621     329.67
 H       4.701535    -1.496091    -1.273686      25.17
 C       6.242447     0.477053    -0.996507      84.78
 O       6.833585     1.763452    -0.793089     276.37
 H       7.136572     1.970526     0.128663      30.48
 H       6.027898     0.176583    -2.119959      28.76
 H       6.934825    -0.398659    -0.526089      28.77
55
name= lig-ACN-Water-frame_444
 C      -2.659912     0.781340    -3.105397      53.05
 H      -2.754456    -0.317079    -3.444558      24.92
 C      -3.562056     2.301571    -1.573830      66.88
 H      -3.862313     2.423357    -0.540950      25.52
 C      -3.204109     3.403225    -2.332714      22.26
 O      -3.387712     4.688229    -1.895036     220.95
 C      -4.431714     5.199989    -0.917066     105.05
 H      -5.484246     4.643301    -0.998243      24.65
 H      -4.430759     6.247081    -1.022864      26.01
 H      -4.405320     4.859454     0.149196      25.93
 C      -2.608180     3.155033    -3.645553      22.80
 O      -2.391640     4.172729    -4.558244     170.01
 H      -2.609769     5.027864    -4.186650      23.22
 C      -2.373527     1.821800    -4.065401      71.48
 H      -1.986267     1.513216    -4.962459      29.82
 C      -3.248051     0.970443    -1.853036      32.68
 C      -3.787910    -0.272003    -1.050233     107.29
 H      -4.399242    -0.879472    -1.712780      27.49
 O      -4.505019    -0.141541     0.161173     177.94
 H      -3.900576    -0.068136     1.018222      22.92
 C      -2.666889    -1.342233    -0.865169      94.48
 H      -2.016801    -1.452764    -1.658136      28.61
 C      -3.139585    -2.646998    -0.381473     119.74
 O      -3.832985    -3.374924    -1.333942     226.39
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 H      -3.474993    -3.412244    -2.168783      31.24
 H      -3.990054    -2.360061     0.358916      25.56
 H      -2.317295    -3.307812     0.192695      26.54
 C       1.787712    -0.736120    -1.080569      41.13
 H       2.463179    -1.227933    -1.801347      20.34
 C       1.426311     1.075003     0.462624      52.99
 H       1.792597     2.107281     1.065016      20.08
 C       0.086723     0.569935     0.749368     -14.82
 O      -0.772178     1.066770     1.756353     206.57
 C      -0.641183     2.433107     2.185084     130.90
 H      -1.481235     2.481129     2.937288      25.03
 H       0.180999     2.737571     2.777035      26.23
 H      -0.863515     2.940791     1.433541      31.29
 C      -0.383712    -0.650636    -0.022711       0.91
 O      -1.797084    -0.787656     0.202394     142.43
 C       0.435338    -1.282022    -0.934104      70.51
 H       0.204617    -2.276958    -1.761888      19.17
 C       2.295236     0.446979    -0.508166      33.27
 C       3.688404     0.964801    -0.957996     103.94
 H       3.716836     0.880129    -2.059843      26.19
 O       3.860815     2.360276    -0.756127     172.72
 H       4.107404     2.656232     0.266189      22.72
 C       4.866067     0.204585    -0.265758      96.93
 H       4.992675     0.221361     0.844989      25.43
 O       4.621015    -1.274480    -0.270377     300.98
 H       4.759313    -1.695990    -1.173206      29.81
 C       6.227650     0.342640    -1.038180      91.32
 O       6.792315     1.746149    -0.822817     239.82
 H       7.116874     1.592750     0.093130      29.29
 H       6.169212     0.320932    -2.218438      27.74
 H       7.087414    -0.377199    -0.724561      28.73
55
name= lig-ACN-Water-frame_445
 C      -2.625355     0.723972    -3.125062      56.98
 H      -2.491443    -0.299048    -3.658188      22.58
 C      -3.545568     2.234181    -1.441291      48.43
 H      -4.167578     2.492432    -0.654945      23.55
 C      -3.143542     3.381656    -2.291600       3.30
 O      -3.374546     4.805733    -1.936241     203.73
 C      -4.475652     5.140006    -0.966577     104.63
 H      -5.371262     4.577946    -1.461641      24.46
 H      -4.757873     6.179688    -0.983719      26.44
 H      -3.951346     4.944561    -0.008211      25.93
 C      -2.692247     3.155951    -3.647595      12.56
 O      -2.389508     4.131680    -4.534190     125.84
 H      -2.746784     5.063395    -4.324521      23.38
 C      -2.478546     1.782339    -4.005075      60.82
 H      -1.993957     1.792254    -4.897488      27.83
 C      -3.244292     0.880080    -1.800301      27.43
 C      -3.767036    -0.385487    -1.046839      87.85
 H      -4.528133    -0.760459    -1.661868      25.86
 O      -4.560544    -0.145263     0.200946     168.39
 H      -4.017955     0.384482     0.896191      26.01
 C      -2.574145    -1.354940    -0.805478     100.11
 H      -2.176476    -1.454091    -1.750893      27.74
 C      -3.175781    -2.738769    -0.268321      98.08
 O      -3.912806    -3.385967    -1.395900     217.58
 H      -3.136209    -3.695305    -1.951542      28.01
 H      -3.860099    -2.610052     0.716523      24.49
 H      -2.290267    -3.434411     0.083900      25.92
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 C       1.784107    -0.755629    -1.122397      47.35
 H       2.479394    -1.345573    -1.714378      25.42
 C       1.428812     1.089041     0.487364      71.94
 H       1.804084     2.106457     0.966132      22.52
 C       0.126513     0.580160     0.697438       1.05
 O      -0.784320     1.016378     1.748109     179.13
 C      -0.697640     2.483418     2.153953     125.97
 H      -1.372919     2.667992     3.016266      26.24
 H       0.269341     2.625015     2.374121      28.51
 H      -0.840679     3.178491     1.499881      31.26
 C      -0.441154    -0.561368     0.030358      -8.23
 O      -1.847822    -0.774040     0.205162     158.39
 C       0.498193    -1.250667    -0.906906      52.32
 H      -0.055404    -2.107301    -1.653065      20.42
 C       2.254627     0.397579    -0.441390       9.52
 C       3.665263     0.985246    -0.910562      95.74
 H       3.732883     0.792859    -1.988570      26.91
 O       3.845550     2.422114    -0.789238     171.38
 H       3.918592     2.560536     0.206112      26.84
 C       4.817112     0.072390    -0.317136      91.01
 H       4.834427     0.702145     0.638530      27.79
 O       4.525869    -1.311282    -0.256330     288.79
 H       4.511341    -1.682212    -1.176212      29.86
 C       6.247430     0.388007    -1.050772      91.70
 O       6.760487     1.661269    -0.826712     224.87
 H       7.037644     1.910321     0.100486      26.41
 H       6.000960     0.265534    -2.192917      27.54
 H       6.824593    -0.508259    -0.702080      29.83
55
name= lig-ACN-Water-frame_446
 C      -2.692242     0.639503    -3.103349      46.79
 H      -2.158421    -0.330177    -3.328843      26.73
 C      -3.509537     2.261499    -1.354748      60.45
 H      -4.129173     2.305636    -0.542583      24.22
 C      -3.220045     3.409200    -2.187841      11.74
 O      -3.354179     4.829412    -2.006410     240.70
 C      -4.448493     5.019087    -1.077065     118.40
 H      -5.376093     4.372991    -1.087995      26.34
 H      -4.661846     6.096045    -1.308097      25.88
 H      -4.331901     4.809027     0.033055      26.45
 C      -2.768891     3.132073    -3.519756      15.34
 O      -2.388308     4.105186    -4.540787     122.77
 H      -2.573308     5.071666    -4.135683      20.89
 C      -2.486799     1.829814    -3.962855      53.28
 H      -2.317035     1.480648    -4.930642      25.35
 C      -3.260617     0.874157    -1.850693      22.22
 C      -3.808538    -0.407573    -1.052411      88.09
 H      -4.429428    -0.947199    -1.648511      26.78
 O      -4.557059    -0.103292     0.170930     170.30
 H      -3.982964     0.269435     0.824631      28.92
 C      -2.692562    -1.482739    -0.789102      68.58
 H      -2.002778    -1.745213    -1.527397      26.93
 C      -3.151673    -2.849491    -0.266003     103.91
 O      -3.920071    -3.399142    -1.394384     141.00
 H      -3.393726    -4.108782    -2.014240      24.84
 H      -3.946574    -2.739123     0.693951      23.87
 H      -2.218327    -3.434575    -0.032222      26.36
 C       1.747785    -0.787191    -1.099644      54.70
 H       2.201593    -1.297382    -1.941478      23.12
 C       1.366755     1.062101     0.475501      67.81
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 H       1.750725     1.875503     1.111679      24.95
 C       0.083195     0.599344     0.795780      21.25
 O      -0.768929     1.077184     1.695855     224.90
 C      -0.668870     2.487191     2.094845     123.03
 H      -1.238607     2.493176     3.024826      27.71
 H       0.250714     2.704299     2.369975      29.35
 H      -1.129099     2.935463     1.339573      30.77
 C      -0.418583    -0.455497    -0.039586      19.98
 O      -1.677424    -0.726617     0.302948      85.16
 C       0.402049    -1.135668    -0.823949      70.29
 H       0.115567    -2.170853    -1.266187      24.10
 C       2.244874     0.408069    -0.472309      12.99
 C       3.582525     0.866225    -0.937110      94.33
 H       3.583417     0.765006    -2.003590      26.84
 O       3.811548     2.450450    -0.743078     194.21
 H       3.969980     2.658946     0.131828      26.64
 C       4.833706     0.115227    -0.352813      96.28
 H       5.087205     0.041657     0.768865      23.64
 O       4.465487    -1.332797    -0.235807     299.83
 H       4.435002    -1.776265    -1.144052      28.63
 C       6.127440     0.315399    -1.021174     105.38
 O       6.778230     1.658995    -0.824425     256.97
 H       6.955867     1.622950     0.157109      28.70
 H       6.125332     0.234099    -2.157396      27.19
 H       6.906898    -0.335997    -0.702392      29.55
55
name= lig-ACN-Water-frame_447
 C      -2.716951     0.725393    -3.061472      70.82
 H      -2.626582    -0.307180    -3.407852      23.46
 C      -3.528281     2.226544    -1.352692      58.08
 H      -3.687701     2.395427    -0.327499      21.76
 C      -3.225576     3.361034    -2.223340      24.29
 O      -3.390515     4.688559    -1.975790     270.09
 C      -4.494988     5.008145    -1.110246     104.64
 H      -5.215659     4.327633    -1.572986      25.81
 H      -4.972516     6.089119    -1.114692      24.63
 H      -4.028078     4.883922    -0.104037      25.84
 C      -2.716310     3.085048    -3.525512       8.42
 O      -2.432588     4.057108    -4.436368     108.08
 H      -2.712242     5.069049    -4.179118      22.62
 C      -2.512358     1.720463    -3.912020      59.56
 H      -2.134484     1.834461    -4.944057      26.03
 C      -3.341938     0.927101    -1.794156      39.06
 C      -3.793048    -0.390916    -1.066506      88.79
 H      -4.473134    -0.801216    -1.677940      28.02
 O      -4.528322    -0.071170     0.094962     223.18
 H      -3.915775    -0.016422     0.856205      26.12
 C      -2.631792    -1.468352    -0.658442      83.41
 H      -2.199827    -1.524680    -1.674749      25.47
 C      -3.128208    -2.941797    -0.309814     103.04
 O      -3.936736    -3.448837    -1.370625     240.22
 H      -3.362010    -3.951521    -1.959082      29.11
 H      -3.925438    -2.954595     0.683116      23.35
 H      -2.340192    -3.626013    -0.000404      26.09
 C       1.676321    -0.737454    -1.103368      50.68
 H       2.362235    -1.228335    -1.785644      21.24
 C       1.434802     1.062098     0.501296      70.76
 H       1.910498     1.817507     1.001534      22.98
 C       0.118468     0.648526     0.753614      30.26
 O      -0.758028     1.145267     1.717976     235.58
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 C      -0.684064     2.508160     2.064129     130.26
 H      -1.257714     2.687608     2.989128      26.03
 H       0.199705     2.998726     2.174377      27.95
 H      -1.040548     3.218505     1.393167      28.42
 C      -0.428843    -0.346331     0.005055     -11.60
 O      -1.758920    -0.828936     0.353496     157.25
 C       0.363774    -1.201904    -0.861337      46.80
 H      -0.060460    -2.085275    -1.233901      20.04
 C       2.158593     0.408469    -0.519147      18.25
 C       3.608039     0.958969    -0.892061      98.25
 H       3.731331     0.770841    -1.960973      27.45
 O       3.736627     2.330311    -0.706319     202.84
 H       4.215766     2.380239     0.141015      26.05
 C       4.751130     0.054652    -0.255468      76.67
 H       4.789982     0.712745     0.770631      24.73
 O       4.452618    -1.373539    -0.279390     314.13
 H       4.607310    -1.707224    -1.238785      27.92
 C       6.186921     0.274866    -1.075660      98.64
 O       6.758605     1.636888    -0.807236     214.18
 H       7.183051     1.761806     0.068294      28.39
 H       6.010723     0.131210    -2.150936      31.22
 H       6.687277    -0.552580    -0.716782      33.61
55
name= lig-ACN-Water-frame_448
 C      -2.828203     0.664205    -3.033787      51.54
 H      -2.996858    -0.254261    -3.518727      25.33
 C      -3.518646     2.263994    -1.309157      57.56
 H      -3.869448     2.625118    -0.304388      19.92
 C      -3.215599     3.207796    -2.272814      18.27
 O      -3.396662     4.637713    -1.941140     209.03
 C      -4.596346     4.949934    -1.088427     106.38
 H      -5.515680     4.418652    -1.115009      27.56
 H      -4.632676     6.104717    -1.445635      23.08
 H      -4.503615     4.804914     0.021464      25.67
 C      -2.682659     3.014940    -3.523641      44.40
 O      -2.462162     4.068935    -4.381136     232.08
 H      -2.909954     4.884286    -4.013553      21.24
 C      -2.439504     1.776048    -3.987779      54.98
 H      -1.913120     1.281003    -4.866707      26.18
 C      -3.333397     0.877914    -1.745215      26.54
 C      -3.739340    -0.384840    -1.037628     108.57
 H      -4.281344    -0.920154    -1.676032      28.82
 O      -4.558962    -0.061196     0.107633     202.49
 H      -3.957821     0.056371     0.961182      23.23
 C      -2.594128    -1.370262    -0.715590      68.47
 H      -1.778239    -1.586632    -1.493942      23.86
 C      -3.136030    -2.950326    -0.281111      88.27
 O      -3.932440    -3.534921    -1.390312     256.51
 H      -3.386985    -3.524799    -2.163117      31.49
 H      -3.767288    -2.831399     0.807397      23.72
 H      -2.220130    -3.469890    -0.189551      26.59
 C       1.614530    -0.737540    -1.197357      44.05
 H       2.222198    -1.474709    -1.748119      22.22
 C       1.515285     1.129072     0.532625      57.92
 H       1.837805     1.976025     0.948002      24.15
 C       0.100173     0.724904     0.710283     -26.13
 O      -0.704499     1.184189     1.754922     169.03
 C      -0.715111     2.744711     2.063753      97.90
 H      -1.217870     2.760888     3.087389      24.01
 H       0.311230     2.702227     2.235962      23.71
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 H      -1.185429     3.141326     1.197754      26.50
 C      -0.534892    -0.514079     0.019352     -16.26
 O      -1.844608    -0.933299     0.414725     179.43
 C       0.307146    -1.206313    -0.882196      57.86
 H      -0.016837    -1.956005    -1.382376      25.27
 C       2.189787     0.456696    -0.528281      13.64
 C       3.550813     0.847690    -0.930242      96.33
 H       3.641784     0.723679    -2.046235      26.70
 O       3.714241     2.282241    -0.623132     155.76
 H       4.183914     2.595527     0.301175      23.16
 C       4.744694     0.064474    -0.292756      83.87
 H       4.950670     0.045858     0.959977      24.46
 O       4.483967    -1.356249    -0.326288     301.21
 H       4.666533    -1.659670    -1.257395      29.39
 C       6.147587     0.277764    -0.971360     109.76
 O       6.752114     1.569927    -0.837998     238.58
 H       6.985955     1.600498     0.129581      28.56
 H       5.966851     0.253874    -2.012840      29.94
 H       6.917305    -0.358395    -0.795917      31.52
55
name= lig-ACN-Water-frame_449
 C      -2.942023     0.649604    -3.139635      69.66
 H      -2.773185    -0.350868    -3.355281      26.13
 C      -3.474491     2.168103    -1.298354      60.83
 H      -4.180996     2.288064    -0.372539      22.06
 C      -3.237450     3.261275    -2.191341       7.78
 O      -3.469632     4.527212    -1.883509     225.12
 C      -4.661218     4.933755    -1.070274     100.41
 H      -5.434680     4.455959    -1.539670      26.84
 H      -4.858826     6.158791    -1.213986      24.04
 H      -4.317296     4.865832    -0.027215      25.64
 C      -2.650234     3.010248    -3.576334     -12.56
 O      -2.468805     4.127715    -4.384142     182.57
 H      -2.669624     4.972968    -4.026796      24.77
 C      -2.369061     1.558040    -3.942464      46.36
 H      -2.104660     1.510912    -5.066623      22.42
 C      -3.289164     0.891259    -1.772682      35.86
 C      -3.749010    -0.410267    -0.988449      93.78
 H      -4.417851    -0.890768    -1.555800      28.42
 O      -4.594086    -0.104310     0.171674     182.58
 H      -4.027612     0.207606     0.938992      25.79
 C      -2.662246    -1.476849    -0.721308      51.86
 H      -2.134179    -1.429999    -1.816295      24.13
 C      -3.082835    -2.797913    -0.400537     114.05
 O      -3.894767    -3.584555    -1.350770     206.11
 H      -3.491272    -3.473570    -2.331955      27.20
 H      -3.848831    -2.914047     0.549410      23.66
 H      -2.241732    -3.367297    -0.102411      26.83
 C       1.559372    -0.692825    -1.186565      44.35
 H       2.133140    -1.083590    -2.069045      21.33
 C       1.341303     1.092608     0.429620      57.60
 H       1.779964     1.893785     0.945730      23.64
 C       0.046026     0.650876     0.724293       3.82
 O      -0.688799     1.280475     1.791689     173.62
 C      -0.646474     2.796326     2.038993     101.56
 H      -1.421202     2.926083     2.883665      24.42
 H       0.197243     3.536962     2.267540      23.86
 H      -1.085574     3.369152     1.143582      26.73
 C      -0.493614    -0.519851     0.143075       8.86
 O      -1.783095    -0.959879     0.485750     101.33
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 C       0.243007    -1.175232    -0.899992      63.95
 H       0.059453    -2.006798    -1.305736      26.38
 C       2.149970     0.348371    -0.525255       2.79
 C       3.599130     0.809728    -0.899223      85.81
 H       3.722100     0.722355    -2.013517      25.07
 O       3.729640     2.313937    -0.584132     193.06
 H       3.966276     2.181613     0.463881      22.64
 C       4.800510    -0.015442    -0.299388      76.30
 H       4.739499     0.445898     0.919209      23.97
 O       4.541502    -1.402518    -0.428915     318.75
 H       4.513641    -1.736539    -1.348152      28.54
 C       6.107592     0.284260    -0.972068     110.86
 O       6.764338     1.579002    -0.816247     275.48
 H       6.899218     1.887587     0.131136      29.62
 H       5.986839     0.074098    -1.969868      30.12
 H       6.571215    -0.514411    -0.529406      30.26
55
name= lig-ACN-Water-frame_450
 C      -2.891580     0.498218    -3.145259      45.12
 H      -2.863473    -0.490615    -3.564211      26.64
 C      -3.488574     2.109798    -1.369059      56.10
 H      -3.857312     2.274220    -0.250484      22.41
 C      -3.200280     3.184099    -2.197502      12.75
 O      -3.528327     4.584770    -1.838609     248.37
 C      -4.687876     4.887914    -1.088778     112.00
 H      -5.575480     4.416936    -1.320033      28.09
 H      -4.829096     6.107818    -1.172317      24.04
 H      -4.703793     4.555242    -0.044857      27.94
 C      -2.651709     3.001285    -3.474695      23.64
 O      -2.434535     4.077056    -4.414204     138.85
 H      -2.642816     4.935585    -3.965743      24.30
 C      -2.436943     1.728451    -3.964833      39.44
 H      -2.111245     1.423328    -5.004309      23.99
 C      -3.322693     0.753645    -1.820633      23.21
 C      -3.868287    -0.393951    -0.945401     108.18
 H      -4.501105    -0.802051    -1.593288      28.43
 O      -4.583697    -0.150369     0.247808     202.06
 H      -4.025357     0.013450     0.992282      27.00
 C      -2.659234    -1.355930    -0.717359      46.39
 H      -1.872921    -1.422302    -1.662652      22.90
 C      -3.094853    -2.894594    -0.394769     108.12
 O      -3.867150    -3.572738    -1.352679     215.14
 H      -3.233461    -3.980204    -2.124358      23.93
 H      -3.765681    -2.626702     0.545045      24.35
 H      -2.207074    -3.418699    -0.102921      25.61
 C       1.505876    -0.702798    -1.251118      49.31
 H       1.956632    -1.170715    -2.183898      24.36
 C       1.249924     1.011531     0.324553      63.16
 H       1.607692     1.931675     0.892803      22.98
 C      -0.008382     0.652722     0.862069      18.92
 O      -0.654377     1.404191     1.813492     214.22
 C      -0.677239     2.839585     1.951070      88.73
 H      -1.490978     2.997096     2.764832      24.18
 H       0.475633     2.907595     2.468940      20.48
 H      -0.929169     3.277510     0.907336      25.50
 C      -0.500806    -0.547520     0.187394       2.63
 O      -1.759585    -1.006150     0.458173     150.30
 C       0.252856    -1.150003    -0.878593      59.96
 H      -0.308954    -1.926865    -1.214503      23.78
 C       2.126436     0.362493    -0.496940      26.07
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 C       3.562601     0.901389    -0.846182     102.53
 H       3.658490     0.831454    -1.985772      22.86
 O       3.761228     2.233869    -0.550100     267.31
 H       4.015144     2.510415     0.355273      23.79
 C       4.690995     0.004033    -0.329757      77.95
 H       4.948371     0.031450     0.964010      22.53
 O       4.589473    -1.497667    -0.495814     306.61
 H       4.569568    -1.648604    -1.479208      27.38
 C       6.198587     0.252634    -0.953723     111.03
 O       6.751132     1.616176    -0.803533     266.87
 H       7.008597     1.659198     0.162064      28.88
 H       6.211579     0.125575    -1.960837      31.39
 H       6.957307    -0.348446    -0.608370      30.58
55
name= lig-ACN-Water-frame_451
 C      -2.760389     0.571924    -3.173819      76.64
 H      -2.937744    -0.358929    -3.769205      24.27
 C      -3.493629     2.039055    -1.414810      49.07
 H      -3.730300     2.309347    -0.313214      18.91
 C      -3.229771     3.261177    -2.170103      15.97
 O      -3.493178     4.558933    -1.854457     256.96
 C      -4.812392     4.786931    -1.030904     100.92
 H      -5.559528     4.471728    -1.628557      27.99
 H      -4.775169     6.008962    -1.033031      24.91
 H      -4.589462     4.546999    -0.016003      27.27
 C      -2.660367     3.055755    -3.469518      22.49
 O      -2.391665     3.986455    -4.376394     198.63
 H      -2.761838     4.940936    -4.093169      22.88
 C      -2.597430     1.667996    -3.914224      51.17
 H      -2.099301     1.727477    -4.881282      25.18
 C      -3.417609     0.721840    -1.870974      30.76
 C      -3.878096    -0.472289    -0.972428      91.60
 H      -4.453314    -1.131463    -1.383823      27.02
 O      -4.571562    -0.176056     0.333696     217.84
 H      -3.880805    -0.024815     1.032436      24.16
 C      -2.626132    -1.405764    -0.695219      56.61
 H      -2.017422    -1.242944    -1.778202      21.54
 C      -3.077015    -2.886736    -0.282302     105.45
 O      -3.859131    -3.578696    -1.398833     216.07
 H      -3.261186    -4.159680    -1.812576      28.05
 H      -3.706734    -3.067499     0.646037      25.55
 H      -2.167362    -3.476511    -0.120556      25.82
 C       1.518164    -0.725433    -1.319778      40.28
 H       2.115289    -1.417762    -1.992232      20.89
 C       1.288286     1.091874     0.449237      48.76
 H       1.767553     2.168655     0.691577      19.12
 C       0.012596     0.637690     0.843889      12.56
 O      -0.753166     1.344395     1.826698     184.24
 C      -0.612991     2.841235     1.877195      86.13
 H      -1.468219     3.275835     2.511272      22.82
 H       0.464468     3.397069     2.400730      21.22
 H      -0.589511     3.447599     0.824980      22.78
 C      -0.536582    -0.503473     0.209399      12.15
 O      -1.864568    -1.045300     0.436329     186.06
 C       0.215095    -1.148942    -0.787506      50.52
 H      -0.003346    -1.956740    -1.555668      19.57
 C       2.065009     0.364858    -0.605557      -3.87
 C       3.471260     0.840640    -0.859865      76.93
 H       3.533688     0.851746    -2.013660      22.72
 O       3.793767     2.279289    -0.496461     216.41
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 H       4.132868     2.147438     0.336951      30.07
 C       4.834540    -0.141545    -0.369309      68.24
 H       4.601902     0.043384     0.924987      23.55
 O       4.595765    -1.499680    -0.559406     330.17
 H       4.791200    -1.932519    -1.463364      25.58
 C       6.249778     0.289067    -0.944755     111.37
 O       6.717221     1.651649    -0.776951     253.78
 H       7.121588     1.838533     0.113286      26.91
 H       6.132587     0.085728    -1.946687      31.84
 H       6.817563    -0.476525    -0.496218      31.04
55
name= lig-ACN-Water-frame_452
 C      -2.864872     0.556699    -3.133042      52.26
 H      -2.531186    -0.492214    -3.531696      22.57
 C      -3.537185     2.097443    -1.376873      65.32
 H      -4.124782     2.056811    -0.456276      21.57
 C      -3.263927     3.205088    -2.166584      26.95
 O      -3.528438     4.542562    -1.775657     306.85
 C      -4.773711     4.741362    -1.047269     113.02
 H      -5.612661     4.301377    -1.543443      25.94
 H      -4.989618     5.853454    -0.831767      24.45
 H      -4.854944     4.145880    -0.173790      27.38
 C      -2.754362     2.978102    -3.454027      15.18
 O      -2.339675     4.012633    -4.377834     139.18
 H      -2.601408     4.945212    -3.939412      21.67
 C      -2.567500     1.739638    -3.975106      62.02
 H      -2.424913     1.512499    -4.975798      25.64
 C      -3.458958     0.755254    -1.898493      18.71
 C      -3.843936    -0.597233    -0.922905      90.41
 H      -4.516993    -0.944058    -1.512663      25.16
 O      -4.513638    -0.205897     0.299873     221.38
 H      -3.884522     0.165623     1.054326      18.82
 C      -2.720827    -1.571368    -0.657411      72.92
 H      -2.042645    -1.865152    -1.658427      19.11
 C      -3.051278    -2.948286    -0.318551     118.89
 O      -3.850362    -3.563344    -1.340671     282.82
 H      -3.301364    -3.813749    -2.091914      29.66
 H      -3.618839    -2.795860     0.585453      25.70
 H      -2.073757    -3.468159    -0.084528      24.64
 C       1.477862    -0.712666    -1.157700      35.61
 H       2.103787    -1.235981    -1.906838      19.81
 C       1.365169     1.084834     0.447856      50.98
 H       1.830711     2.041149     1.085036      15.39
 C       0.016605     0.672798     0.823500      -6.93
 O      -0.817974     1.296168     1.785129     172.36
 C      -0.543517     2.860279     1.813228      47.41
 H      -1.554779     3.229332     2.170044      20.82
 H       0.443806     2.966674     2.677723      17.90
 H      -0.408785     3.028345     0.573155      19.80
 C      -0.576508    -0.510824     0.138178      -7.92
 O      -1.865890    -0.970166     0.480090     151.33
 C       0.253577    -1.196002    -0.851579      59.36
 H      -0.394486    -2.222419    -0.974994      13.09
 C       2.034191     0.461946    -0.581980      35.55
 C       3.568437     0.790251    -0.992951      70.52
 H       3.707905     0.803654    -2.146806      21.88
 O       3.791513     2.240660    -0.437670     224.48
 H       4.084952     2.306981     0.460105      25.01
 C       4.794105    -0.122586    -0.412121      61.38
 H       5.078332     0.094622     0.864521      21.04
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 O       4.614489    -1.546529    -0.585222     300.78
 H       4.712885    -1.692563    -1.604028      25.67
 C       6.207420     0.281642    -0.935491     112.29
 O       6.690076     1.671576    -0.766311     286.43
 H       6.793968     1.832901     0.203519      30.35
 H       6.380723     0.172994    -1.979409      30.53
 H       7.020231    -0.277651    -0.516641      29.80
55
name= lig-ACN-Water-frame_453
 C      -2.959530     0.579296    -3.153882      46.04
 H      -2.642815    -0.537480    -3.396025      22.00
 C      -3.719834     2.034422    -1.317900      40.67
 H      -4.102672     2.370126    -0.418724      19.94
 C      -3.320645     3.180055    -2.149305      -4.27
 O      -3.541116     4.520329    -1.698507     269.92
 C      -4.808024     4.619987    -1.037014     108.75
 H      -5.564803     4.402195    -1.748030      28.07
 H      -4.842416     5.731007    -0.817281      26.54
 H      -4.750007     4.228146    -0.060002      29.33
 C      -2.777205     3.024624    -3.553552      -7.49
 O      -2.335708     4.073429    -4.306387     164.64
 H      -2.461808     4.935745    -3.853807      24.56
 C      -2.569597     1.603406    -4.010156      52.25
 H      -2.192193     1.539571    -4.953362      23.54
 C      -3.391527     0.705298    -1.757797      37.93
 C      -3.850612    -0.516579    -0.990574     103.50
 H      -4.492698    -1.106174    -1.421486      26.92
 O      -4.486359    -0.228901     0.221295     221.78
 H      -3.783097    -0.084549     0.989350      21.12
 C      -2.654729    -1.574904    -0.679055      33.88
 H      -1.922576    -1.416170    -1.605653      21.06
 C      -3.090731    -3.083232    -0.215162     110.79
 O      -3.881288    -3.579042    -1.286537     249.83
 H      -3.319428    -3.559982    -2.186000      25.90
 H      -3.696778    -3.213875     0.602592      25.95
 H      -2.160741    -3.747403    -0.063455      24.26
 C       1.516085    -0.714453    -1.074704      41.69
 H       2.048482    -1.241774    -1.866521      20.03
 C       1.300580     1.059778     0.497307      11.90
 H       1.851153     1.830267     1.266721      18.34
 C      -0.007928     0.625831     0.746152      26.20
 O      -0.765145     1.329741     1.695964     231.09
 C      -0.566192     2.681541     1.738860      84.36
 H      -1.434463     3.323768     2.009300      23.53
 H       0.399372     3.036786     2.611608      21.53
 H       0.071087     3.299622     0.796626      22.09
 C      -0.568618    -0.473086     0.077127      12.11
 O      -1.816269    -0.897596     0.451883     143.57
 C       0.164735    -1.232139    -0.764850      51.91
 H       0.178444    -2.406945    -1.265724      16.08
 C       2.171173     0.446140    -0.561838     -12.22
 C       3.638299     0.884874    -0.924028     104.37
 H       3.749448     0.987472    -2.060323      22.74
 O       3.777118     2.145973    -0.479562     282.76
 H       4.162274     2.047713     0.471230      23.06
 C       4.758993    -0.046877    -0.454293      61.04
 H       4.478211    -0.035913     0.837267      21.02
 O       4.648561    -1.530761    -0.591397     309.45
 H       4.409258    -1.903853    -1.495672      26.32
 C       6.242933     0.310192    -0.994804     102.10
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 O       6.623141     1.683177    -0.772162     245.29
 H       6.926606     1.816657     0.191085      26.24
 H       6.128493     0.035058    -2.061740      29.57
 H       6.778956    -0.477313    -0.439222      29.07
55
name= lig-ACN-Water-frame_454
 C      -2.961549     0.546617    -3.075100      52.11
 H      -3.151625    -0.428286    -3.697911      22.28
 C      -3.770110     2.040666    -1.379272      58.87
 H      -4.023331     2.035309    -0.392868      25.50
 C      -3.382792     3.111259    -2.220622      17.12
 O      -3.496982     4.389016    -1.686514     225.81
 C      -4.860311     4.651980    -0.973343     100.80
 H      -5.723083     4.264211    -1.589923      26.13
 H      -4.933345     5.674120    -0.793728      26.87
 H      -5.006613     4.025864    -0.127823      28.04
 C      -2.797499     2.949587    -3.475234      31.75
 O      -2.342137     4.120274    -4.225423     168.00
 H      -2.678867     4.922100    -3.863553      23.99
 C      -2.652193     1.659597    -3.956449      66.73
 H      -2.179584     1.337672    -4.805201      31.01
 C      -3.409309     0.749204    -1.771319      20.73
 C      -3.778136    -0.590118    -1.024928      94.46
 H      -4.345529    -1.006936    -1.720564      28.02
 O      -4.543659    -0.227823     0.189843     186.35
 H      -3.962495    -0.011043     0.991811      22.55
 C      -2.581808    -1.470363    -0.614675      92.05
 H      -2.003925    -1.850907    -1.512677      24.48
 C      -3.098031    -3.093964    -0.167953      93.37
 O      -3.976636    -3.622070    -1.269923     200.64
 H      -3.284716    -4.064283    -1.976495      24.44
 H      -3.566310    -2.992416     0.689853      27.72
 H      -2.107443    -3.688625    -0.059139      25.00
 C       1.608333    -0.771156    -1.121311      68.25
 H       2.161437    -1.418476    -1.763823      23.18
 C       1.404359     0.983167     0.468805      83.49
 H       1.683179     1.964924     1.012516      22.64
 C       0.032833     0.627942     0.676639       0.49
 O      -0.757819     1.266625     1.568048     170.81
 C      -0.486491     2.751181     1.752130      63.60
 H      -1.561781     3.066186     1.753751      23.19
 H       0.070304     2.926727     2.892081      21.01
 H      -0.075034     3.085736     0.534053      22.97
 C      -0.563697    -0.507215     0.068448      -0.42
 O      -1.872523    -0.870361     0.395390     183.15
 C       0.383195    -1.222491    -0.749809      56.51
 H      -0.281827    -2.113903    -1.399715      21.54
 C       2.141279     0.319659    -0.430394      33.02
 C       3.511577     0.820792    -0.949110      88.32
 H       3.451563     0.837184    -2.090371      24.42
 O       3.828928     2.226235    -0.458848     191.16
 H       4.298499     2.365683     0.525259      20.81
 C       4.752585    -0.084361    -0.439618      81.76
 H       4.983399     0.250338     0.788146      24.48
 O       4.646497    -1.458638    -0.585062     293.93
 H       4.681835    -1.579221    -1.569413      28.55
 C       6.116423     0.300852    -0.964557     105.72
 O       6.595767     1.676464    -0.816271     218.33
 H       7.079958     1.809619     0.067029      28.11
 H       6.250832     0.252598    -2.112981      29.38
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 H       7.007294    -0.319573    -0.634635      29.60
55
name= lig-ACN-Water-frame_455
 C      -2.976216     0.539245    -3.139486      64.45
 H      -2.962699    -0.549076    -3.507095      23.46
 C      -3.702851     1.949222    -1.377342      51.62
 H      -4.237302     2.309335    -0.532295      19.82
 C      -3.473120     3.101331    -2.186350      23.57
 O      -3.573017     4.356336    -1.639953     258.53
 C      -4.844618     4.640103    -0.964326     120.96
 H      -5.665941     4.339139    -1.732196      24.09
 H      -4.897937     5.630989    -0.768354      26.73
 H      -4.776229     4.226387     0.031891      26.25
 C      -2.793694     3.013940    -3.420569      15.92
 O      -2.371894     4.039358    -4.137468     146.88
 H      -2.676638     4.934837    -3.804816      23.96
 C      -2.696463     1.650441    -3.913771      42.18
 H      -2.650092     1.666735    -4.983704      26.69
 C      -3.476869     0.659189    -1.853776      50.62
 C      -3.756017    -0.560274    -0.992698      91.29
 H      -4.380999    -1.234809    -1.454481      28.19
 O      -4.649462    -0.268806     0.119376     190.53
 H      -4.148350     0.003310     0.881698      26.70
 C      -2.661697    -1.631324    -0.663202      88.35
 H      -2.025750    -1.609533    -1.539736      27.09
 C      -3.122283    -2.923580    -0.234454     129.05
 O      -4.009676    -3.657768    -1.171872     221.27
 H      -3.503449    -4.273141    -1.665786      30.33
 H      -3.653299    -2.951125     0.595304      29.57
 H      -2.210439    -3.589620    -0.063529      26.12
 C       1.734620    -0.926275    -1.146926      41.43
 H       2.368794    -1.337254    -1.916159      19.36
 C       1.403647     0.989041     0.493731      72.39
 H       1.901876     1.909391     0.710906      24.61
 C       0.094985     0.608568     0.690805      21.79
 O      -0.789894     1.284112     1.499693     213.54
 C      -0.570753     2.751506     1.720018      85.46
 H      -1.518349     3.346877     1.838160      23.19
 H       0.176365     2.971118     2.704376      23.38
 H       0.318186     3.400034     0.920687      21.18
 C      -0.397551    -0.565409     0.067336       8.86
 O      -1.825616    -0.831493     0.379541     105.85
 C       0.369605    -1.278254    -0.831692      69.94
 H      -0.026086    -2.314817    -1.415703      21.51
 C       2.242744     0.198780    -0.434013     -13.45
 C       3.522239     0.789725    -0.836022      85.65
 H       3.540192     0.873694    -1.917227      25.08
 O       3.831188     2.305333    -0.504468     168.04
 H       4.166682     2.075510     0.501648      24.52
 C       4.774142     0.006750    -0.374746      78.55
 H       4.724668    -0.042315     0.905788      24.76
 O       4.609851    -1.446426    -0.604910     301.35
 H       4.879875    -1.820110    -1.474616      30.03
 C       6.135314     0.372155    -1.077088      95.88
 O       6.601864     1.708846    -0.851898     262.10
 H       6.822320     1.801155     0.121858      27.45
 H       5.880473     0.057682    -2.206324      26.83
 H       6.742799    -0.474130    -0.557879      28.19
55
name= lig-ACN-Water-frame_456
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 C      -3.006892     0.468727    -3.254814      51.54
 H      -2.578159    -0.396578    -3.781332      24.12
 C      -3.729077     1.910040    -1.347690      52.73
 H      -4.153917     1.767576    -0.311218      20.49
 C      -3.457372     3.083825    -2.054793      18.85
 O      -3.644948     4.417812    -1.613716     266.47
 C      -4.830192     4.686303    -0.922585     124.74
 H      -5.866634     4.334569    -1.426482      24.40
 H      -4.854212     5.664839    -0.864890      26.72
 H      -4.972626     4.179968     0.038556      26.92
 C      -2.853963     2.933762    -3.358158      20.72
 O      -2.371242     3.994880    -4.139737     135.75
 H      -2.523854     5.000984    -3.826529      19.55
 C      -2.752551     1.703674    -3.990307      39.63
 H      -2.367590     1.628643    -5.061127      25.87
 C      -3.494295     0.577323    -1.846056       5.83
 C      -3.929921    -0.654384    -1.018011      94.90
 H      -4.456069    -1.142217    -1.772665      24.65
 O      -4.720541    -0.294075     0.101114     199.04
 H      -4.180794    -0.038140     0.868790      24.79
 C      -2.625398    -1.452880    -0.784497      70.33
 H      -2.166430    -1.691249    -1.684687      26.60
 C      -3.169472    -2.945305    -0.184336     107.58
 O      -4.038434    -3.667606    -1.072822     258.56
 H      -3.467994    -3.895362    -1.796407      31.51
 H      -3.635402    -2.635559     0.665790      26.84
 H      -2.250000    -3.517147     0.081686      25.50
 C       1.765457    -1.003373    -1.080652      49.58
 H       2.274621    -1.563678    -1.875588      20.75
 C       1.497599     0.944251     0.422189      63.34
 H       1.757930     1.775195     0.902756      22.11
 C       0.118865     0.572806     0.751798     -23.16
 O      -0.856822     1.404207     1.449331     165.36
 C      -0.555170     2.750044     1.739747      69.87
 H      -1.556333     3.266574     1.737536      22.20
 H      -0.078590     2.717058     2.844785      22.05
 H       0.064755     3.209340     0.582784      20.09
 C      -0.392881    -0.660901     0.065861      -6.09
 O      -1.675936    -0.880334     0.322512     158.10
 C       0.417399    -1.405507    -0.951711      75.74
 H       0.033405    -2.443558    -1.360648      20.61
 C       2.256419     0.191228    -0.436540      33.07
 C       3.696286     0.883405    -0.824388      96.62
 H       3.750748     0.811175    -1.898839      25.32
 O       3.795716     2.216513    -0.515890     245.04
 H       4.059510     2.549429     0.366455      26.03
 C       4.800774    -0.029013    -0.353219      84.32
 H       4.966071     0.206268     0.863693      24.60
 O       4.584584    -1.442063    -0.581239     337.79
 H       4.590896    -1.522606    -1.592410      28.45
 C       6.104961     0.383792    -1.079744      93.18
 O       6.633861     1.744413    -0.910340     243.03
 H       6.941799     1.879727     0.020375      30.12
 H       6.000039     0.459652    -2.308831      26.96
 H       7.068867    -0.299840    -0.961495      27.72
55
name= lig-ACN-Water-frame_457
 C      -3.029701     0.494952    -3.267462      72.71
 H      -3.014481    -0.492108    -3.646347      22.99
 C      -3.777782     1.810492    -1.305501      49.94
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 H      -4.102239     1.976879    -0.201710      18.46
 C      -3.402161     3.058877    -1.959250       4.01
 O      -3.637418     4.411512    -1.634080     224.15
 C      -4.958539     4.782955    -0.796080      82.01
 H      -5.757078     4.278912    -1.559160      23.78
 H      -5.036072     5.760993    -0.646182      27.25
 H      -4.728570     4.352229     0.183708      26.93
 C      -2.919354     2.946003    -3.366803      -7.43
 O      -2.367896     3.954203    -4.155679     159.66
 H      -2.752956     4.876003    -3.803526      18.34
 C      -2.788641     1.651422    -3.994672      58.54
 H      -2.048574     1.616126    -4.899549      25.70
 C      -3.510686     0.623730    -2.015636      50.07
 C      -3.947591    -0.645974    -1.167537      68.53
 H      -4.657204    -1.413223    -1.539803      23.67
 O      -4.772614    -0.322509     0.112421     105.26
 H      -4.106616    -0.139581     0.882584      23.17
 C      -2.628211    -1.491280    -0.762105      86.88
 H      -2.114586    -1.512566    -1.622852      26.70
 C      -3.120096    -2.859846    -0.092440     104.92
 O      -4.038615    -3.656824    -0.998383     182.35
 H      -3.583867    -3.682427    -1.956616      27.21
 H      -3.792231    -2.736042     0.740112      25.42
 H      -2.313208    -3.508696     0.202353      26.35
 C       1.779750    -0.988744    -1.068441      43.67
 H       2.518871    -1.606407    -1.606965      14.71
 C       1.428535     0.909938     0.473941      54.33
 H       1.875892     1.687276     0.821355      21.84
 C       0.118144     0.480980     0.690320      19.29
 O      -0.872013     1.315224     1.328079     144.89
 C      -0.546262     2.767643     1.728836      77.41
 H      -1.543669     3.318559     1.809241      22.58
 H       0.100594     3.057110     2.645685      23.77
 H       0.292837     3.453103     0.862029      21.14
 C      -0.317806    -0.645658    -0.013122       6.51
 O      -1.732929    -1.004380     0.197074     195.36
 C       0.457712    -1.416721    -0.809303      50.63
 H      -0.020107    -2.177848    -1.409989      22.00
 C       2.333476     0.217967    -0.517457       9.70
 C       3.671427     0.769605    -0.900080      81.72
 H       3.766731     0.796218    -1.945142      23.40
 O       3.788764     2.217897    -0.479075     297.24
 H       4.096492     2.072455     0.368283      28.00
 C       4.986368    -0.053496    -0.347920      87.30
 H       5.225847    -0.094466     0.853917      24.22
 O       4.581496    -1.395471    -0.543137     362.62
 H       4.428460    -1.766086    -1.487233      25.41
 C       6.202287     0.420309    -1.156072      80.59
 O       6.671258     1.797611    -0.927945     268.23
 H       7.054334     1.877514    -0.001620      30.40
 H       5.716320     0.349391    -2.295457      27.79
 H       7.016594    -0.435422    -0.989128      28.29
55
name= lig-ACN-Water-frame_458
 C      -3.109703     0.468437    -3.300958      50.20
 H      -3.168346    -0.423010    -3.859816      24.32
 C      -3.729833     1.928792    -1.345119      49.35
 H      -4.296509     1.839868    -0.346242      19.69
 C      -3.432309     3.062546    -2.067995      21.17
 O      -3.674734     4.420980    -1.568506     242.49
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 C      -4.911627     4.752987    -0.753017      99.65
 H      -6.032114     4.366230    -1.102782      23.47
 H      -4.893397     5.791763    -0.909587      25.75
 H      -4.963387     4.387177     0.299203      26.35
 C      -2.918424     2.909614    -3.380439      12.82
 O      -2.425165     3.937923    -4.127439      77.59
 H      -2.598699     4.895379    -3.889678      22.53
 C      -2.703653     1.664101    -3.960747      45.60
 H      -2.515985     1.710924    -5.138465      22.41
 C      -3.707941     0.600533    -1.908815      33.49
 C      -3.907626    -0.624312    -1.123823      94.23
 H      -4.482196    -1.287581    -1.932042      23.36
 O      -4.743132    -0.342632     0.037268     184.56
 H      -4.197671    -0.016252     0.830003      23.23
 C      -2.688274    -1.648779    -0.805193      80.39
 H      -2.285061    -2.056639    -1.627121      26.74
 C      -3.138841    -2.876737    -0.097288     118.58
 O      -4.007623    -3.606071    -0.918707     215.02
 H      -3.404576    -3.960933    -1.722967      27.05
 H      -3.613676    -2.499340     0.876041      25.24
 H      -2.225269    -3.325802     0.178651      26.47
 C       1.851984    -0.963001    -1.076364      55.69
 H       2.346251    -1.562098    -1.868503      19.31
 C       1.500724     0.876282     0.437158      84.67
 H       1.652734     1.754613     0.889972      23.74
 C       0.088794     0.535786     0.604013     -37.51
 O      -0.824155     1.251881     1.253241     150.61
 C      -0.504845     2.729725     1.672403      66.75
 H      -1.504549     3.260766     1.741353      22.28
 H      -0.041106     2.461630     2.600376      23.43
 H       0.140678     3.213793     0.517415      19.92
 C      -0.494912    -0.649308    -0.052340     -11.88
 O      -1.764867    -1.007270     0.184062     159.37
 C       0.552812    -1.424687    -0.739588      51.63
 H       0.282220    -2.286824    -1.187464      25.12
 C       2.252110     0.214459    -0.469616      38.59
 C       3.705400     0.743817    -0.868913      97.37
 H       3.734086     0.640257    -1.912311      25.61
 O       3.800921     2.137647    -0.419947     254.81
 H       4.205730     2.304680     0.448914      26.65
 C       4.991101    -0.018214    -0.419958      75.98
 H       5.085133     0.337329     0.702396      25.87
 O       4.662494    -1.456305    -0.490733     314.09
 H       4.947759    -1.681150    -1.412340      28.85
 C       6.314155     0.427117    -1.248722      88.77
 O       6.724284     1.776341    -0.937940     248.94
 H       6.850174     1.857948     0.076913      29.97
 H       6.181916     0.437765    -2.488923      25.83
 H       7.267070    -0.268454    -1.078328      27.09
55
name= lig-ACN-Water-frame_459
 C      -3.278130     0.514286    -3.245938      65.69
 H      -3.180674    -0.450937    -3.698844      28.38
 C      -3.785635     1.937377    -1.388206      40.65
 H      -4.137497     2.259505    -0.385555      20.16
 C      -3.550795     3.154011    -2.129097      18.92
 O      -3.722988     4.349618    -1.519046     258.90
 C      -4.828221     4.712724    -0.751455     109.13
 H      -5.808859     4.249143    -1.327661      22.40
 H      -4.896640     5.794154    -0.729844      24.19
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 H      -4.556001     4.549297     0.322216      25.21
 C      -2.841546     2.949147    -3.356471       5.05
 O      -2.468021     4.005525    -4.164280     189.54
 H      -2.636546     4.784559    -3.669990      26.58
 C      -2.735489     1.608556    -3.925676      23.54
 H      -2.445183     1.475208    -5.069018      21.60
 C      -3.647630     0.652763    -1.954699      41.70
 C      -3.908829    -0.710590    -1.111954      81.20
 H      -4.759916    -1.339768    -1.697777      22.99
 O      -4.716846    -0.389956    -0.001871     209.60
 H      -4.222522     0.057796     0.662071      27.74
 C      -2.702344    -1.629776    -0.861411      82.70
 H      -2.120515    -1.706715    -1.711782      27.77
 C      -3.127229    -2.902532     0.004705     107.54
 O      -4.019285    -3.656167    -0.883743     185.83
 H      -3.466063    -4.189097    -1.385377      32.93
 H      -3.790509    -2.730535     0.988511      24.25
 H      -2.336300    -3.532696     0.220877      27.80
 C       1.799961    -0.970751    -1.073717      38.75
 H       2.436837    -1.410676    -1.851111      20.71
 C       1.400480     0.917884     0.436196      33.78
 H       1.954743     1.733633     0.908639      18.36
 C       0.061615     0.528597     0.442823      24.06
 O      -0.864011     1.299247     1.245668     192.69
 C      -0.491523     2.520193     1.573339     112.97
 H      -1.429957     3.121125     1.788500      23.81
 H       0.160724     2.820184     2.395388      25.38
 H       0.298139     3.279612     0.703265      22.25
 C      -0.400094    -0.669234    -0.100593       5.93
 O      -1.813444    -0.971159     0.191593     136.07
 C       0.494574    -1.489909    -0.765823      62.78
 H       0.223024    -2.355276    -0.982151      27.28
 C       2.402134     0.178233    -0.449107     -12.69
 C       3.687777     0.808401    -0.833766     110.11
 H       3.641648     0.988312    -1.857863      23.52
 O       3.823571     2.107032    -0.396110     255.07
 H       4.181493     2.038907     0.613572      21.46
 C       4.981494    -0.030467    -0.532120      89.00
 H       5.330741     0.163973     0.550088      25.64
 O       4.867738    -1.481319    -0.423762     294.89
 H       4.818325    -1.914118    -1.306120      27.78
 C       6.363147     0.412233    -1.277723      80.53
 O       6.791494     1.762389    -0.932746     221.53
 H       6.986842     1.846788     0.052999      29.19
 H       6.237802     0.432683    -2.485292      26.36
 H       7.134706    -0.397348    -0.907158      28.53
55
name= lig-ACN-Water-frame_460
 C      -3.313332     0.519289    -3.270131      48.93
 H      -3.339713    -0.502123    -3.706224      25.58
 C      -3.894028     1.942174    -1.378370      51.62
 H      -4.039449     1.925886    -0.351074      21.52
 C      -3.590109     3.054536    -2.147803      10.04
 O      -3.637350     4.358732    -1.593523     231.33
 C      -4.798569     4.689476    -0.704472      98.95
 H      -5.796113     4.078164    -0.916803      24.79
 H      -5.015029     5.815607    -0.866007      23.74
 H      -4.666137     4.291578     0.322198      26.60
 C      -2.856807     2.978367    -3.399029       7.76
 O      -2.474000     4.052310    -4.204861     227.51
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 H      -2.625758     4.974905    -3.975631      21.88
 C      -2.843219     1.680606    -3.942272      45.16
 H      -2.068210     1.541732    -4.761101      25.39
 C      -3.619957     0.618396    -1.840255      11.11
 C      -3.982249    -0.659818    -1.187891      73.38
 H      -4.447397    -1.510604    -1.929020      24.50
 O      -4.729971    -0.440962     0.070155     153.17
 H      -4.101553    -0.136144     0.785544      23.37
 C      -2.644055    -1.575446    -0.712239      83.21
 H      -2.188409    -1.872384    -1.645936      26.56
 C      -3.114787    -2.931833    -0.041880      96.76
 O      -4.078026    -3.786114    -0.846620     191.88
 H      -3.487658    -4.130280    -1.569974      30.82
 H      -3.726646    -2.469707     0.910419      23.95
 H      -2.248975    -3.387960     0.352043      27.74
 C       1.800091    -1.013131    -1.064422      66.68
 H       2.416694    -1.707411    -1.608653      20.02
 C       1.452530     0.897436     0.334496      65.97
 H       1.618621     1.855204     0.968343      17.44
 C       0.054329     0.576064     0.445815      -2.54
 O      -0.906186     1.182606     1.165084     154.60
 C      -0.430443     2.662211     1.587936      70.94
 H      -1.379324     3.197837     1.731273      23.03
 H       0.211052     2.411692     2.387431      23.85
 H      -0.071298     2.945299     0.320170      20.12
 C      -0.451942    -0.693316    -0.108006       1.94
 O      -1.758503    -0.891012     0.165929     204.96
 C       0.454631    -1.540239    -0.853830      44.87
 H       0.133723    -2.292527    -1.397699      21.97
 C       2.269712     0.133171    -0.387138      39.90
 C       3.687471     0.780416    -0.942255      76.68
 H       3.607745     0.850255    -1.948363      26.78
 O       3.874674     2.188978    -0.306643     175.08
 H       4.203657     2.213824     0.750050      21.25
 C       5.109783    -0.055070    -0.523218      88.08
 H       5.155719     0.326969     0.518787      26.73
 O       5.069115    -1.500062    -0.408304     272.92
 H       4.645674    -1.772431    -1.265127      26.28
 C       6.324132     0.392871    -1.254776     101.28
 O       6.878570     1.733110    -0.939128     179.75
 H       7.110847     1.776019     0.009481      31.08
 H       6.222017     0.307567    -2.411640      27.73
 H       7.136622    -0.422428    -0.998116      29.84
55
name= lig-ACN-Water-frame_461
 C      -3.235325     0.562425    -3.240838      62.41
 H      -3.187750    -0.353260    -3.901121      27.06
 C      -3.913459     1.862399    -1.306609      42.89
 H      -4.391473     2.068642    -0.447916      22.83
 C      -3.525496     3.077574    -2.110951       1.23
 O      -3.620089     4.394597    -1.655372     220.39
 C      -4.759944     4.589097    -0.682251     105.34
 H      -5.667149     4.079563    -1.148773      25.78
 H      -4.896078     5.784017    -0.721812      25.19
 H      -4.381850     4.526624     0.358835      26.23
 C      -3.036247     3.000779    -3.445407     -13.74
 O      -2.452994     4.018168    -4.236185      79.18
 H      -2.686396     4.859911    -3.811875      24.54
 C      -2.831045     1.700546    -3.970966      32.30
 H      -2.525990     1.600092    -5.030273      17.58
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 C      -3.733826     0.597927    -1.929581      36.80
 C      -3.891278    -0.687855    -1.023395      79.03
 H      -4.709244    -1.220697    -1.765562      23.19
 O      -4.769352    -0.490964     0.103689     161.75
 H      -4.158979    -0.336438     0.950516      23.23
 C      -2.678707    -1.584176    -0.747963      85.11
 H      -1.972483    -1.824246    -1.619305      23.81
 C      -3.178031    -2.908580    -0.060664     103.22
 O      -4.005266    -3.855156    -0.796088     154.02
 H      -3.626838    -3.925262    -1.805302      28.81
 H      -3.861134    -2.811419     0.942753      23.46
 H      -2.309708    -3.533231     0.134676      25.42
 C       1.785308    -1.163052    -1.006351      44.07
 H       2.440897    -1.695157    -1.676513      21.21
 C       1.353848     0.939025     0.331160      55.03
 H       1.957426     1.943979     0.525719      15.26
 C       0.067148     0.444137     0.480450      19.27
 O      -0.925260     1.254025     1.155171     156.64
 C      -0.482112     2.627674     1.503540     102.36
 H      -1.248564     3.144048     2.068433      24.98
 H       0.329070     2.718023     2.167918      26.43
 H       0.116907     3.519103     0.675183      22.64
 C      -0.404726    -0.686319    -0.174453      21.15
 O      -1.776418    -0.838904     0.164634     187.28
 C       0.409853    -1.465823    -0.960822      87.36
 H       0.065727    -2.303744    -1.521003      22.20
 C       2.322596     0.102400    -0.515320      15.07
 C       3.736328     0.730390    -0.831982      91.04
 H       3.767583     0.962030    -1.778975      24.84
 O       3.891953     2.182609    -0.342510     173.72
 H       4.221110     2.120294     0.664864      23.84
 C       5.058884     0.020762    -0.389559      85.64
 H       5.294528     0.229866     0.644808      27.36
 O       5.200708    -1.494288    -0.435409     225.48
 H       5.120507    -1.857254    -1.392511      27.13
 C       6.398336     0.395603    -1.267212      92.77
 O       6.970645     1.681164    -0.969829     228.22
 H       6.949849     1.869840     0.004454      31.44
 H       6.101459     0.482761    -2.330750      27.26
 H       7.216236    -0.395646    -1.093524      30.03
55
name= lig-ACN-Water-frame_462
 C      -3.144869     0.536404    -3.229702      53.82
 H      -2.932598    -0.529547    -3.560186      25.23
 C      -3.892372     1.957882    -1.395067      59.71
 H      -4.347250     1.918444    -0.467443      24.05
 C      -3.487608     3.085451    -2.067852      20.51
 O      -3.668883     4.400320    -1.656685     256.85
 C      -4.637285     4.587176    -0.713623     108.63
 H      -5.544098     3.962667    -0.854296      27.14
 H      -5.089043     5.759383    -0.720916      24.74
 H      -4.325648     4.135038     0.240991      28.46
 C      -3.079866     2.969078    -3.463070      -8.71
 O      -2.495966     3.960693    -4.201821      74.08
 H      -2.698819     4.974388    -4.078205      19.19
 C      -2.871555     1.677843    -4.015734      60.74
 H      -2.688378     1.572109    -5.038014      19.75
 C      -3.755143     0.617364    -1.929273      19.28
 C      -3.965043    -0.690562    -1.039584      82.37
 H      -4.448391    -1.656337    -1.552524      25.47
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 O      -4.775383    -0.520704     0.168674     165.16
 H      -4.291035     0.025792     0.910692      23.28
 C      -2.736153    -1.606862    -0.777217      78.76
 H      -2.445223    -1.747530    -1.923214      26.02
 C      -3.142415    -2.977129    -0.024884     108.37
 O      -3.940947    -3.866387    -0.832923     161.83
 H      -3.483060    -3.869781    -1.722218      28.95
 H      -3.696528    -2.641898     0.978454      24.87
 H      -2.132206    -3.312416     0.359047      26.12
 C       1.873137    -1.156240    -1.033288      57.39
 H       2.456125    -1.867070    -1.634436      20.65
 C       1.436658     0.854645     0.171580      73.74
 H       1.538804     1.931547     0.536314      21.91
 C       0.099234     0.528637     0.559012       1.89
 O      -0.856968     1.365308     1.125781     177.16
 C      -0.470876     2.647630     1.525567     108.81
 H      -1.404320     2.960060     1.942193      25.28
 H       0.396472     2.538326     2.096442      25.90
 H      -0.699147     3.166083     0.331252      22.42
 C      -0.486617    -0.664367    -0.153105     -11.84
 O      -1.825391    -0.876026     0.126362     132.81
 C       0.406670    -1.444223    -1.046892      70.42
 H      -0.034478    -2.447845    -1.416246      21.04
 C       2.312749     0.092694    -0.515375      43.89
 C       3.781049     0.715274    -0.727795      99.55
 H       3.854903     0.599551    -1.674916      27.45
 O       3.892200     2.082814    -0.405005     270.34
 H       3.932726     2.235917     0.551685      26.81
 C       5.174890    -0.044225    -0.312549      92.00
 H       5.290915     0.150451     0.723099      27.77
 O       5.239095    -1.441873    -0.445016     276.25
 H       5.147365    -1.675242    -1.421183      26.97
 C       6.368732     0.449194    -1.229504      86.77
 O       7.072237     1.708524    -0.994989     255.07
 H       7.180207     1.813732     0.015825      30.87
 H       6.073058     0.429915    -2.252811      28.19
 H       7.044721    -0.431686    -1.067544      29.02
55
name= lig-ACN-Water-frame_463
 C      -3.117903     0.439804    -3.181494      41.28
 H      -2.786434    -0.532367    -3.642278      21.21
 C      -3.923416     1.921422    -1.423253      56.92
 H      -4.182149     2.194421    -0.389160      21.95
 C      -3.507351     3.105791    -2.177106      13.74
 O      -3.638159     4.416367    -1.724118     204.01
 C      -4.676250     4.540533    -0.597592      96.91
 H      -5.552674     4.031258    -0.940366      26.03
 H      -4.785356     5.818465    -0.586207      23.48
 H      -4.229539     4.374391     0.399541      26.07
 C      -2.974533     2.901620    -3.440494       7.46
 O      -2.553349     3.971462    -4.220152     178.64
 H      -3.088799     4.827800    -3.893007      19.02
 C      -2.951804     1.594988    -4.014110      59.04
 H      -2.263271     1.556956    -4.770783      30.35
 C      -3.658249     0.615494    -1.881861      31.72
 C      -4.118939    -0.718753    -1.087161      79.32
 H      -4.971726    -1.002783    -1.860116      22.90
 O      -4.795981    -0.495530     0.185989     210.90
 H      -4.148752    -0.142757     0.832866      25.84
 C      -2.804297    -1.602135    -0.773951      89.76
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 H      -2.054070    -1.955169    -1.660976      22.85
 C      -3.027774    -2.924690    -0.012046     106.07
 O      -3.841020    -3.849041    -0.881748     190.06
 H      -3.260510    -4.178385    -1.510812      33.02
 H      -3.776604    -2.707874     0.821607      25.32
 H      -2.146621    -3.595648     0.327394      24.70
 C       1.799259    -1.115198    -1.122882      65.79
 H       2.529199    -1.879138    -1.491319      20.78
 C       1.406445     0.915642     0.174701      40.95
 H       1.894561     1.798558     0.479110      23.61
 C       0.061450     0.507019     0.397316      36.37
 O      -0.801952     1.290222     1.120674     169.95
 C      -0.532183     2.754026     1.481122     110.19
 H      -1.100665     3.190229     2.297408      25.92
 H       0.423129     3.007364     1.900012      26.93
 H      -0.218024     3.635567     0.597900      23.99
 C      -0.452264    -0.646241    -0.149987      29.27
 O      -1.828428    -0.931872     0.054048     186.62
 C       0.441950    -1.386104    -0.902585      65.28
 H       0.111592    -2.368724    -1.555484      21.80
 C       2.407003     0.013492    -0.458674      -6.74
 C       3.842273     0.549810    -0.782048      93.66
 H       3.908872     0.601650    -1.726954      27.71
 O       3.870015     2.030193    -0.455322     228.17
 H       4.050851     2.151394     0.464885      26.01
 C       5.242649    -0.024902    -0.240151      99.10
 H       5.541037     0.174273     0.734208      27.71
 O       5.210061    -1.463498    -0.439101     319.80
 H       4.780157    -1.748160    -1.262255      25.48
 C       6.390923     0.473283    -1.161023      94.50
 O       7.134201     1.776900    -0.995488     224.69
 H       7.475750     1.862648    -0.063397      30.84
 H       6.016603     0.542737    -2.104431      29.44
 H       7.204394    -0.248239    -1.187955      29.24
55
name= lig-ACN-Water-frame_464
 C      -3.132778     0.399101    -3.137000      61.06
 H      -3.033220    -0.625556    -3.546487      25.04
 C      -3.876416     1.937439    -1.407272      49.60
 H      -4.433251     1.955765    -0.384292      21.20
 C      -3.587182     3.028584    -2.210838      12.29
 O      -3.659686     4.397177    -1.726072     193.51
 C      -4.630132     4.572223    -0.581524     100.35
 H      -5.604816     4.092526    -0.716428      25.97
 H      -4.939508     5.814787    -0.615084      22.79
 H      -4.166965     4.103131     0.335548      24.84
 C      -2.931800     2.863660    -3.495132      12.75
 O      -2.618010     3.978072    -4.266102     133.84
 H      -2.930812     4.850951    -3.874827      21.48
 C      -2.801050     1.506572    -3.960913      49.34
 H      -2.515145     1.308813    -4.958234      26.18
 C      -3.606748     0.568265    -1.825329      25.27
 C      -4.105872    -0.638559    -1.081780      71.99
 H      -4.894079    -1.414691    -1.700029      22.13
 O      -4.843399    -0.455160     0.130585     198.45
 H      -4.274847    -0.416811     0.900483      26.03
 C      -2.768024    -1.690281    -0.844041      47.14
 H      -2.417585    -1.788797    -2.032438      23.52
 C      -3.083766    -2.949958    -0.044411     112.64
 O      -3.740695    -3.835293    -0.900800     198.79
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 H      -3.010168    -4.148639    -1.562319      27.67
 H      -3.545419    -2.858539     0.930450      25.67
 H      -1.935544    -3.173324     0.204301      23.90
 C       1.812558    -1.090585    -1.067148      58.36
 H       2.240921    -1.728573    -1.896408      23.68
 C       1.509134     0.899475     0.204524      56.69
 H       1.739785     1.731396     0.678948      24.37
 C       0.101216     0.642403     0.283780     -37.38
 O      -0.803361     1.358549     1.173493     137.41
 C      -0.425438     2.817461     1.451145      86.99
 H      -1.339711     2.947497     2.045674      24.01
 H       0.541074     2.664495     1.857672      23.85
 H      -0.919482     3.326606     0.400026      22.28
 C      -0.492713    -0.655503    -0.222800     -28.87
 O      -1.807225    -0.870826     0.077943     103.14
 C       0.482636    -1.499542    -0.860779      52.35
 H      -0.074203    -2.499907    -1.438432      21.56
 C       2.405604     0.009783    -0.424670      32.77
 C       3.894918     0.542636    -0.792432     108.93
 H       3.952800     0.334795    -1.719019      30.18
 O       3.848955     1.956738    -0.512962     204.56
 H       4.347691     2.098354     0.366863      25.02
 C       5.217547    -0.041076    -0.258314      97.24
 H       5.217059     0.121999     0.740880      29.87
 O       5.174599    -1.524512    -0.372194     275.77
 H       4.949031    -1.754531    -1.309574      27.75
 C       6.525203     0.525087    -1.181905      91.98
 O       7.139936     1.842663    -0.976637     231.48
 H       7.233190     1.975772     0.003015      28.83
 H       6.165970     0.612183    -2.117245      28.98
 H       7.156799    -0.350783    -1.120671      31.18
55
name= lig-ACN-Water-frame_465
 C      -3.110794     0.392048    -3.134778      42.10
 H      -3.274319    -0.605304    -3.562439      24.62
 C      -3.850293     1.863953    -1.358521      56.77
 H      -4.489738     2.082561    -0.381569      19.93
 C      -3.565324     3.019192    -2.177822      14.78
 O      -3.752905     4.310242    -1.736788     248.48
 C      -4.562944     4.569983    -0.639124     103.91
 H      -5.536396     4.062716    -0.830674      26.21
 H      -4.671677     5.809371    -0.436742      24.04
 H      -4.097914     4.216331     0.363803      26.13
 C      -2.986077     2.848192    -3.490857     -11.34
 O      -2.668866     3.925685    -4.334519     191.79
 H      -2.783258     4.752323    -3.911760      26.23
 C      -2.628657     1.470726    -3.941683      43.44
 H      -2.628797     1.336166    -5.025900      21.54
 C      -3.662360     0.584023    -1.821451      36.97
 C      -3.963815    -0.718931    -1.008180      87.07
 H      -4.542590    -1.375839    -1.906236      22.94
 O      -4.904785    -0.416312     0.089164     191.47
 H      -4.333167     0.038994     0.811045      23.88
 C      -2.811833    -1.531222    -0.801377      73.95
 H      -2.210508    -1.860486    -1.822685      21.64
 C      -2.984893    -2.921285    -0.080773     106.83
 O      -3.697354    -3.925608    -0.916784     144.99
 H      -3.221310    -3.886371    -1.902961      25.82
 H      -3.651433    -2.705138     0.679406      26.16
 H      -2.044708    -3.547456     0.298794      23.07
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 C       1.835677    -1.187039    -1.037748      54.83
 H       2.582718    -1.582037    -1.768815      16.95
 C       1.518282     0.874605     0.309492      56.40
 H       1.950102     1.665359     0.756241      21.09
 C       0.082959     0.658120     0.330157      16.63
 O      -0.727521     1.395376     1.130402     229.96
 C      -0.481754     2.720732     1.388688     123.62
 H      -0.963929     3.277112     2.215596      24.12
 H       0.444163     3.209065     1.686705      24.64
 H      -0.294711     3.449878     0.329342      22.99
 C      -0.416942    -0.542163    -0.228566       1.01
 O      -1.812760    -0.826985     0.040131     141.55
 C       0.410969    -1.550261    -0.863952      70.07
 H       0.200548    -2.745292    -1.318319      17.03
 C       2.413377     0.038826    -0.441980       7.60
 C       3.811201     0.533972    -0.837675     104.48
 H       3.840377     0.518290    -1.795045      27.00
 O       3.900183     1.940863    -0.615265     225.05
 H       4.101971     2.184840     0.429635      21.57
 C       5.202097    -0.121074    -0.312890      88.19
 H       5.412589     0.142419     0.636814      28.20
 O       5.167121    -1.523100    -0.310421     285.78
 H       5.193547    -1.889854    -1.250232      29.33
 C       6.535183     0.496255    -1.179969      95.77
 O       7.113426     1.871723    -0.926833     212.57
 H       7.149667     2.020832     0.065737      28.55
 H       6.385522     0.381249    -2.185216      29.64
 H       7.432309    -0.046192    -0.947507      30.27
55
name= lig-ACN-Water-frame_466
 C      -3.092927     0.403036    -3.157526      58.65
 H      -2.895943    -0.550429    -3.690637      22.84
 C      -3.873262     1.881391    -1.337573      48.67
 H      -4.145459     2.062456    -0.218107      17.82
 C      -3.495621     2.945678    -2.148350      23.40
 O      -3.777256     4.259966    -1.851609     203.99
 C      -4.566320     4.541563    -0.614740      93.29
 H      -5.690212     4.291887    -0.634694      27.37
 H      -4.570224     5.707981    -0.767691      26.16
 H      -3.976948     4.107746     0.330765      27.17
 C      -2.965895     2.786132    -3.459894      15.91
 O      -2.727536     3.831176    -4.378979     214.26
 H      -2.947314     4.710479    -3.946713      23.93
 C      -2.681088     1.546852    -3.904462      58.41
 H      -1.933617     1.443281    -4.766643      23.51
 C      -3.656143     0.545654    -1.882088      30.26
 C      -4.025854    -0.662882    -1.057869      49.09
 H      -4.812582    -1.494394    -1.587690      21.08
 O      -4.910310    -0.410987     0.040554     146.64
 H      -4.426713     0.118155     0.811003      24.14
 C      -2.581206    -1.536692    -0.688446      74.36
 H      -2.193241    -1.528121    -1.826238      23.24
 C      -2.986174    -2.913958    -0.101448     105.14
 O      -3.673251    -3.976559    -0.921943     170.89
 H      -3.287045    -3.984326    -1.880754      27.64
 H      -3.580061    -2.841228     0.725875      25.99
 H      -1.909043    -3.202298     0.332064      24.03
 C       1.837216    -1.213921    -0.984071      61.23
 H       2.330762    -2.136607    -1.272183      18.72
 C       1.533680     0.832526     0.368781      70.85
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 H       1.919215     1.760109     0.803922      16.87
 C       0.211352     0.555693     0.435879     -13.34
 O      -0.726917     1.370329     1.111557     180.16
 C      -0.381949     2.876668     1.323292      61.67
 H      -1.315131     2.986185     1.916924      21.92
 H       0.516038     2.590188     1.734586      22.47
 H      -0.800213     3.410868     0.229914      20.58
 C      -0.410657    -0.612406    -0.256214      -1.67
 O      -1.731070    -0.708476     0.048295     185.80
 C       0.505199    -1.429536    -0.846888      68.29
 H      -0.202426    -2.439465    -1.171908      19.52
 C       2.315894    -0.026626    -0.463699      31.28
 C       3.779634     0.520637    -0.929249      88.71
 H       3.765248     0.353092    -1.869681      25.54
 O       3.978204     2.022730    -0.684997     181.28
 H       4.020251     2.090980     0.364116      21.57
 C       5.214380    -0.070123    -0.399086      91.83
 H       5.300787     0.224252     0.553746      27.08
 O       5.203783    -1.557618    -0.277316     297.80
 H       4.981266    -1.921611    -1.209493      25.04
 C       6.548461     0.419090    -1.122848      87.77
 O       7.000457     1.858113    -0.923465     243.99
 H       7.173249     1.984525     0.074154      29.42
 H       6.484690     0.359982    -2.179087      29.56
 H       7.134521    -0.374222    -0.681553      30.52
55
name= lig-ACN-Water-frame_467
 C      -3.034947     0.396078    -3.199200      61.63
 H      -2.649920    -0.651644    -3.358628      24.87
 C      -3.808796     1.800811    -1.377758      58.32
 H      -4.185839     1.866062    -0.347992      20.49
 C      -3.505931     2.941511    -2.158144      27.51
 O      -3.834903     4.267208    -1.910107     250.06
 C      -4.526207     4.579035    -0.677128     108.45
 H      -5.560862     4.007540    -0.776940      24.40
 H      -4.564483     5.650598    -0.411231      25.82
 H      -3.934057     4.006977     0.244361      24.45
 C      -2.940207     2.808770    -3.444021      25.24
 O      -2.797048     3.785473    -4.367125     196.58
 H      -3.043776     4.754145    -4.005614      20.41
 C      -2.671122     1.490209    -3.911978      53.06
 H      -1.915235     1.405934    -4.820220      25.80
 C      -3.690645     0.540820    -1.909101      33.19
 C      -4.026997    -0.686527    -1.087729      73.70
 H      -4.395249    -1.535070    -1.936179      23.45
 O      -4.903355    -0.395996     0.049287     180.27
 H      -4.279946    -0.274106     0.812616      25.46
 C      -2.636809    -1.524210    -0.800013      55.76
 H      -2.017296    -1.884425    -1.699286      24.34
 C      -2.927885    -2.959128    -0.036301     108.18
 O      -3.607392    -3.914813    -0.879440     208.87
 H      -2.979040    -4.112784    -1.536880      31.86
 H      -3.525989    -2.730559     0.788868      26.61
 H      -1.983759    -3.592738     0.227303      23.95
 C       1.858329    -1.284079    -0.903738      32.16
 H       2.593801    -1.945960    -1.355771      21.47
 C       1.616697     0.771397     0.324200      53.80
 H       2.041005     1.821069     0.703706      21.84
 C       0.201587     0.531095     0.571676      38.37
 O      -0.744767     1.348147     1.081849     178.99
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 C      -0.404779     2.818730     1.287363     104.12
 H      -1.049635     3.337748     1.994568      25.01
 H       0.422050     3.378600     1.771377      24.71
 H      -0.106409     3.468982     0.206458      24.40
 C      -0.336320    -0.522217    -0.116875      15.45
 O      -1.695485    -0.632042     0.097327     119.43
 C       0.413162    -1.504006    -0.866603      69.38
 H       0.203255    -2.522456    -1.479263      19.75
 C       2.500115     0.000515    -0.442155      20.98
 C       3.836815     0.554934    -1.002896     108.47
 H       3.811624     0.513294    -1.957871      29.69
 O       3.995586     2.006688    -0.761820     159.56
 H       4.397890     2.151098     0.081254      28.53
 C       5.119111    -0.040376    -0.400456     107.96
 H       5.123188     0.204519     0.544726      29.76
 O       5.233874    -1.535495    -0.300969     295.17
 H       5.038433    -1.911458    -1.201383      27.63
 C       6.518491     0.369433    -1.058706     106.63
 O       6.864970     1.739297    -0.930968     268.92
 H       6.946091     1.945588     0.068830      27.04
 H       6.494166     0.128087    -2.159324      27.31
 H       7.430520    -0.138861    -0.727918      29.22
55
name= lig-ACN-Water-frame_468
 C      -2.972398     0.299309    -3.137150      52.61
 H      -2.778751    -0.701644    -3.676853      22.51
 C      -3.804047     1.819278    -1.393525      57.31
 H      -4.400674     1.938125    -0.560949      22.28
 C      -3.557469     2.982621    -2.201570       8.29
 O      -3.866955     4.325845    -1.936144     234.68
 C      -4.499772     4.516135    -0.704130     111.55
 H      -5.661061     4.179285    -0.660150      24.19
 H      -4.619532     5.536480    -0.721098      26.88
 H      -3.832751     4.141461     0.311041      23.75
 C      -2.958354     2.728651    -3.483848      -0.68
 O      -2.849297     3.853022    -4.360511     153.40
 H      -3.047799     4.674048    -3.829679      23.03
 C      -2.558451     1.455746    -3.952517      54.62
 H      -2.486885     1.335232    -5.128329      23.83
 C      -3.642671     0.491980    -1.973935      38.84
 C      -3.889444    -0.799039    -1.154938      74.47
 H      -4.813064    -1.397309    -1.656951      22.73
 O      -4.824414    -0.446745     0.032524     160.55
 H      -4.368808    -0.495365     0.853262      27.88
 C      -2.672150    -1.561028    -0.745331      87.29
 H      -2.203247    -1.577895    -1.732215      25.09
 C      -2.829272    -2.915244     0.035328     111.86
 O      -3.554669    -3.824763    -0.849764     233.80
 H      -2.985191    -4.123164    -1.584916      30.43
 H      -3.485431    -2.872165     0.911830      25.48
 H      -1.802279    -3.152433     0.466814      26.45
 C       1.935980    -1.231888    -0.880934      56.14
 H       2.347178    -1.819563    -1.684298      23.68
 C       1.686752     0.850503     0.327874      57.21
 H       2.180883     1.939968     0.662171      21.45
 C       0.346247     0.577345     0.596624     -34.96
 O      -0.695242     1.468517     1.162307     132.16
 C      -0.379664     2.815623     1.274448      99.23
 H      -1.377463     3.184100     1.457349      24.01
 H       0.487344     2.558006     1.904854      21.74
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 H      -0.318393     3.115340     0.021736      24.21
 C      -0.349852    -0.696620    -0.065075     -40.79
 O      -1.799625    -0.663566     0.066664     105.96
 C       0.529412    -1.530885    -0.802486      68.07
 H      -0.087528    -2.307679    -1.296933      21.68
 C       2.522002    -0.087019    -0.425157      24.18
 C       3.894981     0.560222    -1.041312     101.79
 H       3.917143     0.340755    -1.981668      30.57
 O       3.990271     1.984531    -0.862779     209.87
 H       4.202521     2.108034     0.054508      27.41
 C       5.176288    -0.145094    -0.340227     111.23
 H       5.159393     0.153800     0.587987      31.97
 O       5.198112    -1.500312    -0.351544     291.45
 H       5.256246    -1.848982    -1.250711      30.78
 C       6.459265     0.293821    -1.036156      98.18
 O       6.742286     1.726146    -0.924342     237.69
 H       7.009042     1.866733     0.034228      27.16
 H       6.374263     0.020056    -2.166914      28.32
 H       7.104867    -0.396345    -0.447047      30.31
55
name= lig-ACN-Water-frame_469
 C      -2.869494     0.299140    -3.241715      51.47
 H      -3.058613    -0.741694    -3.684367      23.55
 C      -3.900818     1.822061    -1.481238      58.40
 H      -4.308312     1.883434    -0.557393      22.71
 C      -3.561425     2.905161    -2.291428      18.93
 O      -3.853107     4.262418    -1.987823     198.66
 C      -4.557276     4.589810    -0.658583      92.54
 H      -5.554979     3.890488    -0.620563      25.22
 H      -4.663976     5.584257    -0.549029      27.33
 H      -3.730281     4.144914     0.224311      23.89
 C      -2.962972     2.758023    -3.579835      11.56
 O      -2.882948     3.888567    -4.327801     183.21
 H      -3.134056     4.657549    -3.861017      26.40
 C      -2.604573     1.433078    -3.983909      54.84
 H      -2.248695     1.297478    -5.087046      22.23
 C      -3.500901     0.485322    -1.896687       8.78
 C      -3.982649    -0.795905    -1.072378      92.77
 H      -4.215319    -1.705459    -1.865755      23.06
 O      -4.739964    -0.537232     0.014413     214.92
 H      -4.103601    -0.232790     0.764978      22.37
 C      -2.581754    -1.599673    -0.699584      79.05
 H      -2.097065    -2.026086    -1.545270      24.47
 C      -2.788490    -2.831310     0.058094     122.25
 O      -3.468692    -3.783184    -0.799424     163.48
 H      -2.984119    -3.689220    -1.769506      26.07
 H      -3.364334    -2.647854     1.031954      25.46
 H      -1.805312    -3.303794     0.271652      25.15
 C       1.922094    -1.220506    -0.993191      34.46
 H       2.527243    -1.847473    -1.652736      16.79
 C       1.687147     0.872745     0.349781      44.24
 H       2.102601     1.982854     0.744583      16.78
 C       0.250499     0.517025     0.503305      11.96
 O      -0.592734     1.320308     1.187817     188.20
 C      -0.337436     2.848234     1.212398     106.98
 H      -1.140704     3.349692     1.644815      24.27
 H       0.226006     3.449339     2.019767      23.10
 H       0.290041     3.434216     0.326341      22.43
 C      -0.328539    -0.637211     0.092440      16.04
 O      -1.773328    -0.693664     0.036573     143.30
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 C       0.570926    -1.527163    -0.660381      75.12
 H       0.337804    -2.356667    -1.184165      23.99
 C       2.517391     0.020425    -0.426083      25.55
 C       3.898008     0.390782    -0.960757     109.06
 H       3.926258     0.202014    -1.917911      25.94
 O       3.956388     1.937336    -0.944682     205.38
 H       4.142307     2.253802     0.026191      20.98
 C       5.153061    -0.105637    -0.305196     115.91
 H       5.266932     0.060930     0.664320      27.43
 O       5.130336    -1.630565    -0.365158     291.18
 H       4.863683    -1.885209    -1.304483      26.40
 C       6.468735     0.273353    -0.986652     103.37
 O       6.682106     1.721083    -0.910300     249.96
 H       7.044185     1.908597    -0.023958      30.63
 H       6.470515     0.059059    -2.177433      30.01
 H       7.446194    -0.211052    -0.702763      30.75
55
name= lig-ACN-Water-frame_470
 C      -2.920700     0.353825    -3.182361      61.20
 H      -2.521831    -0.629884    -3.582702      22.75
 C      -3.905721     1.695821    -1.555222      63.02
 H      -4.363442     1.939649    -0.642849      20.95
 C      -3.612937     2.876834    -2.312734      16.88
 O      -3.887730     4.204950    -1.960705     239.32
 C      -4.506483     4.539388    -0.716325     117.94
 H      -5.612383     4.013701    -0.583470      25.60
 H      -4.776160     5.530449    -0.831489      26.32
 H      -3.812573     4.324196     0.361288      23.47
 C      -2.995601     2.766276    -3.595869      10.74
 O      -2.861201     3.920506    -4.383335     211.04
 H      -3.249148     4.691048    -3.860030      21.99
 C      -2.673408     1.475275    -4.110415      60.01
 H      -1.972245     1.395325    -4.947983      24.28
 C      -3.440497     0.453774    -1.925041      47.32
 C      -3.744459    -0.810426    -1.156772      68.49
 H      -4.731197    -1.280816    -1.728776      19.71
 O      -4.719992    -0.628575     0.081870     122.79
 H      -4.288414     0.042598     0.767434      23.64
 C      -2.456625    -1.562013    -0.744080      82.09
 H      -1.948651    -1.647562    -1.631639      24.45
 C      -2.723577    -2.892974     0.126597     109.54
 O      -3.430951    -3.776882    -0.750450     208.81
 H      -3.145692    -3.665150    -1.735772      28.00
 H      -3.436780    -2.705762     1.060898      23.65
 H      -1.798622    -3.280135     0.529997      26.43
 C       1.885345    -1.088175    -0.946689      50.13
 H       2.481733    -1.836328    -1.502204      16.89
 C       1.590819     0.777509     0.323198      61.14
 H       1.939291     1.755589     0.917577      17.08
 C       0.299018     0.563539     0.499057      11.27
 O      -0.523767     1.371864     1.270397     232.96
 C      -0.289050     2.912224     1.243071      65.01
 H      -1.260047     3.115904     1.028364      23.09
 H       0.471963     2.899371     2.078478      19.98
 H      -0.000201     2.953023     0.128430      23.94
 C      -0.266066    -0.697880     0.021504       2.33
 O      -1.645626    -0.645439     0.108531     141.29
 C       0.569578    -1.585998    -0.594675      53.50
 H       0.195227    -2.456344    -0.815436      21.95
 C       2.451233     0.036302    -0.486208      53.72
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 C       3.849063     0.434583    -0.895634     101.78
 H       3.925516     0.051845    -1.820339      26.85
 O       3.912970     1.829243    -0.995954     199.70
 H       4.526121     2.145991    -0.168629      17.73
 C       5.178469    -0.315114    -0.229729      88.02
 H       5.149407    -0.019513     0.758295      25.47
 O       5.049232    -1.713990    -0.312480     344.87
 H       4.859105    -2.028783    -1.274475      25.08
 C       6.542406     0.353966    -1.023838      81.91
 O       6.695902     1.757972    -0.883602     272.02
 H       6.756931     1.938922     0.100873      29.97
 H       6.270293     0.032691    -2.161203      28.81
 H       7.336837    -0.286815    -0.499072      29.03
55
name= lig-ACN-Water-frame_471
 C      -2.819307     0.385654    -3.306256      54.39
 H      -2.166918    -0.471321    -3.450178      24.34
 C      -3.901770     1.745659    -1.514685      43.23
 H      -4.542291     1.666532    -0.605395      21.25
 C      -3.675586     2.847930    -2.332635      24.09
 O      -3.909283     4.123235    -1.946250     225.08
 C      -4.537615     4.503589    -0.760956     106.77
 H      -5.569087     3.918199    -0.562366      24.34
 H      -4.653352     5.553838    -0.868617      25.44
 H      -3.666354     4.425535     0.224068      23.10
 C      -3.086619     2.789867    -3.654087      18.41
 O      -2.823385     3.912924    -4.433492     156.15
 H      -3.050753     4.853733    -3.987048      22.94
 C      -2.713637     1.528930    -4.083561      65.03
 H      -2.352599     1.381960    -5.045945      24.65
 C      -3.481944     0.447500    -1.982791      34.81
 C      -3.647277    -0.800201    -1.073293      71.40
 H      -4.020820    -1.782621    -1.816517      22.79
 O      -4.634567    -0.684487     0.090527     184.64
 H      -4.289268    -0.139279     0.813962      25.82
 C      -2.327749    -1.552406    -0.680544      95.59
 H      -1.787117    -1.855729    -1.479441      26.93
 C      -2.635967    -2.866565     0.083526     108.82
 O      -3.436023    -3.847279    -0.710366     205.28
 H      -2.969796    -3.962871    -1.487568      33.38
 H      -3.433465    -2.492594     0.887613      23.09
 H      -1.771488    -3.282857     0.513916      27.10
 C       1.844248    -1.256079    -0.933312      60.01
 H       2.464903    -1.837890    -1.656358      17.95
 C       1.671456     0.885350     0.367516      49.30
 H       2.241966     1.716848     0.806333      19.41
 C       0.265309     0.554141     0.588386      10.85
 O      -0.524286     1.432109     1.373091     242.32
 C      -0.289848     2.791387     1.135527     122.59
 H      -1.015599     3.414105     1.469908      25.97
 H       0.233243     3.388874     1.964235      22.93
 H       0.344442     3.130916     0.342354      27.25
 C      -0.291339    -0.562758    -0.026190       3.31
 O      -1.616413    -0.652264     0.185748     170.98
 C       0.593731    -1.691661    -0.609083      57.68
 H       0.276450    -2.668452    -0.906726      21.50
 C       2.388832     0.021072    -0.485960      31.90
 C       3.829000     0.329144    -0.930674      89.25
 H       3.926762     0.075314    -1.917971      25.45
 O       3.943699     1.820447    -1.024785     184.70
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 H       4.451910     2.168564    -0.255973      20.08
 C       5.171939    -0.339807    -0.201107      80.97
 H       5.320357    -0.214862     0.856931      25.12
 O       5.005823    -1.795476    -0.237790     301.44
 H       5.058586    -2.060857    -1.223498      27.21
 C       6.434847     0.263657    -0.958896      92.93
 O       6.735395     1.810609    -0.821638     228.61
 H       6.828239     2.008817     0.179147      28.64
 H       6.602505     0.268987    -2.165128      25.73
 H       7.492341    -0.180891    -0.714600      26.97
55
name= lig-ACN-Water-frame_472
 C      -2.728597     0.376881    -3.254994      64.79
 H      -2.552341    -0.545534    -3.746137      24.74
 C      -3.923402     1.671550    -1.535856      61.43
 H      -4.406165     1.940791    -0.515710      19.80
 C      -3.721163     2.845749    -2.345003      24.49
 O      -3.933949     4.154703    -1.997097     223.44
 C      -4.558155     4.507459    -0.715599     107.38
 H      -5.547213     3.888458    -0.506756      25.98
 H      -4.924347     5.594847    -0.744269      25.44
 H      -3.798799     4.145791     0.235050      24.10
 C      -3.182957     2.814934    -3.660318      -8.58
 O      -2.804803     3.903341    -4.469804     154.51
 H      -3.007142     4.742648    -3.937266      24.60
 C      -2.706223     1.534378    -4.133530      32.18
 H      -2.446952     1.577736    -5.142473      22.71
 C      -3.468039     0.446614    -2.024545      27.65
 C      -3.611320    -0.869540    -1.060487      74.19
 H      -4.257500    -1.736591    -1.779505      23.63
 O      -4.490926    -0.723982     0.015498     186.20
 H      -3.977163    -0.477479     0.784621      26.53
 C      -2.285783    -1.546336    -0.636466     101.00
 H      -1.760571    -1.620368    -1.468096      28.91
 C      -2.645734    -2.862975     0.082138     118.40
 O      -3.399866    -3.889232    -0.688625     180.72
 H      -2.757676    -4.326030    -1.332156      29.22
 H      -3.169398    -2.741275     1.126638      25.49
 H      -1.742988    -3.322386     0.315877      27.99
 C       1.911805    -1.353390    -0.924092      55.18
 H       2.514720    -2.073288    -1.525940      20.62
 C       1.718272     0.894292     0.378713      65.86
 H       2.096157     1.779212     0.678333      23.69
 C       0.385796     0.642904     0.690296      -4.17
 O      -0.538164     1.374158     1.411926     193.06
 C      -0.263122     2.916286     1.164498      85.19
 H      -1.221410     3.184302     1.021646      26.55
 H       0.621048     3.036584     1.827760      22.14
 H      -0.082472     2.927806     0.138877      30.24
 C      -0.230086    -0.536700     0.034394     -31.10
 O      -1.637340    -0.702174     0.285976     172.62
 C       0.513011    -1.619921    -0.607067      57.26
 H      -0.040973    -2.542078    -1.048086      23.31
 C       2.418396    -0.103158    -0.463916      24.73
 C       3.843473     0.266111    -0.958004      93.47
 H       3.908452    -0.129570    -1.941946      28.03
 O       4.006637     1.802062    -1.047662     190.93
 H       4.217350     2.042005    -0.180489      27.51
 C       5.091745    -0.274137    -0.242583      82.33
 H       5.033299     0.132307     0.809162      26.42
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 O       5.039339    -1.835537    -0.202143     231.21
 H       4.781733    -2.137684    -1.137376      28.42
 C       6.444029     0.291304    -0.904261      84.89
 O       6.738321     1.748677    -0.729526     198.02
 H       7.177360     1.851377     0.156315      27.23
 H       6.059298     0.018739    -2.004032      27.50
 H       7.255681    -0.450001    -0.457384      28.68
55
name= lig-ACN-Water-frame_473
 C      -2.810629     0.387777    -3.260391      56.82
 H      -2.671793    -0.596532    -3.620295      26.37
 C      -3.916083     1.684461    -1.610819      45.03
 H      -4.247924     1.631834    -0.494423      21.64
 C      -3.761108     2.883180    -2.374513       9.43
 O      -4.013543     4.273369    -1.974734     199.44
 C      -4.608333     4.426029    -0.681781     111.38
 H      -5.575369     3.868119    -0.660030      26.91
 H      -4.723113     5.610364    -0.653068      24.75
 H      -3.801885     4.299208     0.311514      24.25
 C      -3.126693     2.732946    -3.684231      19.49
 O      -2.840990     3.900081    -4.432863     184.27
 H      -3.205569     4.687957    -4.069959      26.22
 C      -2.715573     1.515947    -4.124029      70.06
 H      -2.094207     1.313392    -5.002963      25.52
 C      -3.365115     0.384198    -1.967610      32.73
 C      -3.612040    -0.887324    -1.229919      81.52
 H      -4.290102    -1.674855    -1.990473      23.58
 O      -4.410591    -0.713580     0.010407     126.25
 H      -3.830433    -0.447986     0.852214      23.43
 C      -2.376135    -1.575362    -0.703877      67.74
 H      -1.733128    -1.781159    -1.444616      26.87
 C      -2.557314    -3.009208     0.112732     110.64
 O      -3.364923    -3.890852    -0.674239     160.33
 H      -2.681550    -4.348999    -1.379722      26.51
 H      -3.169542    -2.808178     1.032920      26.00
 H      -1.596512    -3.364985     0.376523      26.94
 C       1.858525    -1.337256    -0.812381      47.22
 H       2.398714    -2.127596    -1.363819      25.17
 C       1.776001     0.766616     0.309926      61.03
 H       2.238925     1.614208     0.522995      25.96
 C       0.391097     0.547996     0.698119      10.38
 O      -0.476286     1.418485     1.416320     203.60
 C      -0.322748     2.858891     1.134895     126.66
 H      -1.033329     3.440270     1.639509      26.44
 H       0.374042     3.449513     1.667539      27.18
 H      -0.062198     2.946321     0.139270      29.79
 C      -0.194554    -0.588824     0.236865       9.46
 O      -1.573134    -0.705619     0.409934     107.86
 C       0.520064    -1.436678    -0.636679      70.53
 H      -0.158088    -2.403766    -1.078999      19.92
 C       2.530905    -0.173700    -0.409901      25.62
 C       3.844047     0.302387    -1.019197     109.86
 H       3.893262     0.064425    -2.090238      28.76
 O       4.032456     1.683650    -1.039900     223.49
 H       4.316398     2.073051    -0.203042      26.16
 C       5.010539    -0.276255    -0.215088      94.12
 H       4.839117    -0.096866     0.910844      25.92
 O       5.099387    -1.716703    -0.181513     261.84
 H       4.868450    -2.042813    -1.075034      31.34
 C       6.353144     0.262881    -0.848927      89.32
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 O       6.757064     1.584025    -0.676507     248.32
 H       7.052380     1.737575     0.250141      27.50
 H       6.600895     0.200522    -2.009442      24.91
 H       7.262804    -0.416111    -0.477210      27.78
55
name= lig-ACN-Water-frame_474
 C      -2.910373     0.274862    -3.334977      70.46
 H      -2.263792    -0.524194    -3.617600      26.48
 C      -3.855677     1.731647    -1.560485      59.42
 H      -4.531775     1.863597    -0.667877      23.45
 C      -3.753295     2.921146    -2.390246      13.24
 O      -4.071511     4.214769    -1.990039     225.57
 C      -4.654926     4.418250    -0.642425      99.54
 H      -5.614080     3.911414    -0.460437      26.16
 H      -4.974768     5.607952    -0.464720      24.00
 H      -3.862088     3.826830     0.083258      24.40
 C      -3.069770     2.807526    -3.617139      12.24
 O      -2.881619     3.882804    -4.392777     188.55
 H      -3.273284     4.674502    -3.956271      24.98
 C      -2.659237     1.422961    -4.065578      40.67
 H      -2.136681     1.453406    -5.107313      23.35
 C      -3.360470     0.506246    -2.005292      31.17
 C      -3.604280    -0.862529    -1.166649      65.77
 H      -4.064408    -1.746195    -1.936675      23.61
 O      -4.438669    -0.681693    -0.011245     143.43
 H      -3.737560    -0.203655     0.578349      27.37
 C      -2.280890    -1.741447    -0.668077      60.77
 H      -1.618931    -1.786714    -1.518874      26.67
 C      -2.504886    -2.989228     0.090480     127.42
 O      -3.318811    -3.948675    -0.687453     197.23
 H      -2.970673    -4.135699    -1.546682      30.46
 H      -3.033105    -2.814997     0.997535      27.67
 H      -1.569335    -3.510084     0.364026      26.43
 C       1.906061    -1.353222    -0.782082      34.39
 H       2.340138    -2.049221    -1.506780      23.50
 C       1.754830     0.753186     0.362938      76.78
 H       2.176644     1.701258     0.618663      24.84
 C       0.446932     0.542782     0.751230       3.02
 O      -0.351887     1.464533     1.411090     234.59
 C      -0.346792     2.852181     1.163346     123.19
 H      -1.313721     3.071519     1.539362      26.35
 H       0.635909     3.060172     1.481523      25.33
 H      -0.573023     3.221578     0.142162      29.02
 C      -0.268570    -0.653491     0.315818      10.54
 O      -1.650313    -0.768884     0.434955     105.17
 C       0.476012    -1.428947    -0.580686      58.32
 H       0.205745    -2.558875    -1.219380      20.61
 C       2.566356    -0.177900    -0.412400      21.34
 C       3.853495     0.228337    -1.027563      96.80
 H       3.890165    -0.192521    -2.067332      27.60
 O       4.012293     1.706685    -1.050298     150.97
 H       4.366998     1.943978    -0.075327      20.94
 C       5.059925    -0.286112    -0.239717      95.77
 H       5.049343     0.247669     0.783876      26.26
 O       5.128013    -1.664484    -0.192758     261.33
 H       5.236680    -2.005585    -1.108749      30.99
 C       6.393846     0.111527    -0.796279      88.28
 O       6.797564     1.538685    -0.616626     270.68
 H       6.831708     1.789775     0.361670      26.83
 H       6.125658    -0.191807    -1.886349      27.00
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 H       7.139673    -0.629172    -0.270317      28.17
55
name= lig-ACN-Water-frame_475
 C      -2.849236     0.288987    -3.304806      54.95
 H      -2.664518    -0.757481    -3.643962      26.37
 C      -3.846172     1.776937    -1.505769      53.90
 H      -4.422587     1.798924    -0.616205      21.79
 C      -3.681094     2.899630    -2.307141      17.66
 O      -4.176548     4.157612    -2.000606     195.98
 C      -4.698787     4.317784    -0.632372     108.18
 H      -5.669225     3.884267    -0.645081      25.21
 H      -4.610938     5.573233    -0.523593      23.63
 H      -3.985237     4.015291     0.321586      23.86
 C      -3.025649     2.727728    -3.548399      21.83
 O      -2.885489     3.904337    -4.390769     146.37
 H      -3.037334     4.842859    -3.930310      20.28
 C      -2.646803     1.547161    -4.062982      54.32
 H      -2.320109     1.492685    -5.173368      22.75
 C      -3.437358     0.408510    -2.008791      -6.71
 C      -3.511953    -0.873157    -1.079625      83.82
 H      -4.325768    -1.479565    -1.756101      25.78
 O      -4.477276    -0.625793    -0.026633     161.57
 H      -4.282297    -0.196822     0.770535      28.92
 C      -2.232680    -1.624231    -0.619856      89.73
 H      -1.551877    -1.782343    -1.525630      24.35
 C      -2.508201    -3.079479     0.060877     119.95
 O      -3.305655    -4.000727    -0.712731     217.81
 H      -3.046109    -3.858577    -1.609953      33.18
 H      -3.015788    -2.869400     0.910289      28.72
 H      -1.462938    -3.447555     0.316777      26.50
 C       1.890384    -1.336533    -0.840561      47.45
 H       2.453187    -1.979630    -1.502161      22.59
 C       1.793880     0.791652     0.450164      51.04
 H       2.192970     1.848362     0.777146      21.93
 C       0.419160     0.486908     0.754279      17.01
 O      -0.312588     1.397523     1.442166     174.19
 C      -0.360609     2.909520     1.188109     102.77
 H      -0.925589     3.345854     2.021654      26.05
 H       0.366544     3.567991     1.336973      27.96
 H      -0.651337     2.914231     0.042977      26.47
 C      -0.238458    -0.666258     0.242519     -15.27
 O      -1.727566    -0.869611     0.391955     164.96
 C       0.561209    -1.627227    -0.471349      55.82
 H      -0.298651    -2.523699    -0.932681      18.35
 C       2.468922    -0.126991    -0.386460      15.83
 C       3.908009     0.236488    -0.965833      97.49
 H       3.992243    -0.130620    -2.059516      24.95
 O       3.947965     1.734911    -1.105010     206.66
 H       4.169766     2.245980    -0.155170      20.01
 C       5.138366    -0.235775    -0.210973      92.37
 H       4.959952    -0.076140     0.928942      25.76
 O       5.113669    -1.783934    -0.172693     212.85
 H       5.207606    -2.072019    -1.144589      29.95
 C       6.533045     0.085643    -0.781021     104.25
 O       6.830249     1.454887    -0.636252     260.45
 H       7.112818     1.683371     0.309717      27.49
 H       6.764840    -0.017673    -1.882891      28.28
 H       7.313340    -0.623522    -0.300499      28.88
55
name= lig-ACN-Water-frame_476
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 C      -2.819596     0.424595    -3.230297      68.20
 H      -2.894566    -0.506310    -3.853700      25.84
 C      -3.824811     1.586260    -1.456613      59.96
 H      -4.100697     1.671061    -0.484170      23.80
 C      -3.619934     2.847347    -2.215045      23.90
 O      -4.238426     4.096931    -1.969582     230.83
 C      -4.730931     4.295032    -0.650762     111.42
 H      -5.749438     3.989168    -0.491765      27.76
 H      -4.913912     5.551414    -0.478564      24.35
 H      -4.025115     3.657238     0.056031      25.33
 C      -3.002474     2.865307    -3.543857       6.87
 O      -2.852150     3.866918    -4.378983     157.51
 H      -3.148732     4.805423    -3.976949      21.63
 C      -2.663308     1.494186    -4.044462      51.79
 H      -2.297199     1.419455    -5.074208      24.61
 C      -3.414606     0.406765    -1.937449      57.49
 C      -3.632307    -0.832057    -1.088073      89.34
 H      -3.874363    -1.848581    -1.721036      24.39
 O      -4.568182    -0.575842     0.038525     149.01
 H      -3.863884    -0.350856     0.680679      27.09
 C      -2.372161    -1.596429    -0.630150      52.75
 H      -1.699670    -1.629364    -1.617281      25.92
 C      -2.537840    -3.076475     0.017959     112.76
 O      -3.290722    -4.037584    -0.775513     138.65
 H      -3.080647    -4.064484    -1.840138      25.08
 H      -3.046397    -3.034039     0.882604      28.80
 H      -1.547786    -3.644958     0.262572      25.95
 C       1.833821    -1.298299    -0.856976      34.52
 H       2.412663    -1.992532    -1.463011      21.58
 C       1.750575     0.724558     0.494039      47.39
 H       2.320639     1.702750     1.023094      21.02
 C       0.397572     0.513163     0.714297       9.52
 O      -0.362202     1.417736     1.581674     187.23
 C      -0.370265     2.861975     1.203734      90.60
 H      -1.124846     3.246726     1.949833      24.29
 H       0.625942     3.001665     1.054304      26.50
 H      -1.059504     3.112956     0.186908      25.38
 C      -0.223584    -0.717201     0.196971     -10.46
 O      -1.515793    -0.844801     0.407805     116.03
 C       0.601167    -1.741177    -0.376076      69.74
 H       0.413966    -2.869745    -0.773401      25.95
 C       2.510796    -0.097740    -0.413267       4.82
 C       3.884720     0.361486    -0.906119      91.73
 H       3.979409    -0.100963    -1.999210      25.22
 O       3.874112     1.761560    -1.151655     192.30
 H       4.259993     2.185710    -0.265293      21.37
 C       5.199241    -0.445545    -0.160874      72.67
 H       5.365091    -0.020050     0.944092      25.10
 O       5.075728    -1.854324    -0.174675     254.38
 H       4.861674    -2.161925    -1.107356      28.04
 C       6.697027     0.071118    -0.773723      93.81
 O       6.933673     1.482064    -0.669695     273.78
 H       7.052756     1.744789     0.301155      25.56
 H       6.641080    -0.305692    -1.798734      28.69
 H       7.457112    -0.479235    -0.138492      28.21
55
name= lig-ACN-Water-frame_477
 C      -2.884258     0.347600    -3.212263      59.53
 H      -2.463688    -0.658788    -3.573145      25.52
 C      -3.770192     1.699297    -1.370545      53.25
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 H      -4.337265     1.735831    -0.493738      22.59
 C      -3.633884     2.798789    -2.202045      18.83
 O      -4.252023     4.011266    -1.944411     224.84
 C      -4.816162     4.267555    -0.608358     107.02
 H      -5.780725     3.747321    -0.556266      25.94
 H      -4.687605     5.501482    -0.371158      23.69
 H      -4.132128     3.887007     0.269556      25.78
 C      -3.004449     2.773430    -3.456905      21.96
 O      -2.808473     3.904527    -4.393002     201.13
 H      -3.239010     4.764161    -4.103240      23.25
 C      -2.672493     1.599686    -3.979509      60.04
 H      -2.361046     1.492189    -4.946600      27.07
 C      -3.331845     0.379081    -1.898369      26.87
 C      -3.752027    -0.900704    -1.069903      72.10
 H      -4.613445    -1.395428    -1.746709      23.31
 O      -4.551647    -0.536561     0.086961     100.90
 H      -4.134992    -0.403460     1.041305      23.25
 C      -2.382821    -1.649618    -0.593456      50.34
 H      -1.736657    -1.762861    -1.621611      24.84
 C      -2.601044    -3.037315    -0.053750     115.20
 O      -3.314944    -4.060825    -0.882952     170.03
 H      -2.690086    -4.154371    -1.708137      27.98
 H      -3.076246    -2.986504     0.859033      27.25
 H      -1.459648    -3.279263     0.123834      24.19
 C       1.970439    -1.281564    -0.834415      49.19
 H       2.430701    -1.922650    -1.596655      22.44
 C       1.727850     0.673744     0.509331      31.35
 H       2.332057     1.569770     1.173009      21.35
 C       0.348503     0.534889     0.733713      -1.39
 O      -0.428836     1.338224     1.630610     182.41
 C      -0.412717     2.733317     1.226727      96.33
 H      -0.444073     3.387453     2.137641      23.94
 H       0.506795     3.212382     1.010007      25.72
 H      -1.105295     2.971419     0.124956      23.46
 C      -0.118105    -0.703030     0.237135     -49.23
 O      -1.502592    -0.833239     0.426151      90.34
 C       0.689406    -1.682472    -0.354417      85.22
 H       0.090636    -2.525590    -0.615366      26.81
 C       2.506452    -0.105208    -0.399886      33.95
 C       3.904639     0.281120    -0.902489      73.97
 H       4.002428    -0.139635    -2.023076      24.64
 O       3.869251     1.816656    -1.122137     163.65
 H       4.183621     2.292001    -0.341382      23.72
 C       5.326234    -0.441035    -0.153498      74.41
 H       5.097504    -0.333083     1.042865      23.82
 O       5.009944    -1.899132    -0.207623     254.17
 H       4.853690    -2.125134    -1.149528      28.26
 C       6.689115    -0.040975    -0.714871     102.61
 O       7.033957     1.530561    -0.728894     279.97
 H       7.086843     1.800800     0.220953      27.20
 H       6.836135    -0.220102    -1.744573      27.81
 H       7.518762    -0.564845    -0.228136      27.52
55
name= lig-ACN-Water-frame_478
 C      -2.850723     0.282681    -3.184681      53.71
 H      -2.414341    -0.685928    -3.563562      23.50
 C      -3.698814     1.701005    -1.337310      62.14
 H      -4.429630     1.766633    -0.507364      21.76
 C      -3.691878     2.859819    -2.179306      23.33
 O      -4.265838     4.026477    -1.854441     232.10
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 C      -4.839805     4.218667    -0.551095     113.02
 H      -5.915864     3.889637    -0.534099      24.30
 H      -5.182553     5.381921    -0.707332      23.60
 H      -4.205071     3.799406     0.319237      25.24
 C      -3.020985     2.819319    -3.483290       4.33
 O      -2.799298     3.870046    -4.319662     218.12
 H      -3.001406     4.716630    -3.938892      26.36
 C      -2.654531     1.442595    -3.941340      46.23
 H      -2.242449     1.507113    -4.866968      26.36
 C      -3.378127     0.452027    -1.806265      29.06
 C      -3.703576    -0.808250    -0.965004      83.15
 H      -4.249103    -1.676342    -1.593463      24.39
 O      -4.548990    -0.494855     0.178567     169.37
 H      -3.824362    -0.169109     0.831356      26.10
 C      -2.421652    -1.663402    -0.676983      64.89
 H      -1.655367    -1.726322    -1.639486      24.13
 C      -2.613750    -3.096401    -0.040142     113.41
 O      -3.274130    -3.994702    -0.982863     217.89
 H      -2.783463    -4.255682    -1.688237      31.57
 H      -3.297336    -3.039206     0.813688      26.19
 H      -1.707388    -3.744983     0.304985      25.06
 C       2.053259    -1.382758    -0.827513      30.32
 H       2.634770    -1.964623    -1.579901      18.02
 C       1.791956     0.740580     0.559344      61.78
 H       2.280424     1.816384     0.989603      22.01
 C       0.409803     0.484163     0.843179      -2.36
 O      -0.426775     1.216417     1.592256     213.30
 C      -0.400508     2.721464     1.279581      83.23
 H      -0.867613     3.203696     2.175035      23.12
 H       0.500785     2.807357     0.642930      24.57
 H      -1.486205     2.728049     0.583018      22.31
 C      -0.196127    -0.670250     0.302228     -24.48
 O      -1.648026    -0.907825     0.372084      99.76
 C       0.698245    -1.581507    -0.427223      59.22
 H       0.338693    -2.424585    -0.882490      26.49
 C       2.580735    -0.103497    -0.312909     -33.37
 C       4.013557     0.298722    -0.886036      86.72
 H       4.042656    -0.087748    -2.052847      22.80
 O       3.929405     1.769701    -1.078589     238.39
 H       4.127086     2.207768    -0.281454      24.26
 C       5.191773    -0.379859    -0.159726      75.17
 H       5.348231    -0.071412     1.046013      23.50
 O       4.980576    -1.883042    -0.294017     270.20
 H       5.215495    -2.145770    -1.223993      29.15
 C       6.716033     0.023154    -0.707496     107.45
 O       7.071630     1.416932    -0.757964     300.14
 H       7.393711     1.755272     0.099942      29.11
 H       6.706125    -0.351485    -1.665631      31.33
 H       7.391674    -0.539321    -0.117479      29.22
55
name= lig-ACN-Water-frame_479
 C      -2.804077     0.305728    -3.023416      65.72
 H      -2.815676    -0.683243    -3.483062      25.87
 C      -3.758483     1.735516    -1.369502      58.66
 H      -4.052265     1.818024    -0.248551      18.85
 C      -3.665666     2.848425    -2.194485      15.72
 O      -4.266989     4.130271    -1.788070     215.65
 C      -4.969991     4.233238    -0.524066     108.97
 H      -5.758312     3.404453    -0.366706      24.16
 H      -5.116557     5.353788    -0.213469      24.23
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 H      -4.208045     3.992919     0.301753      25.90
 C      -3.049514     2.680174    -3.457343      33.37
 O      -2.787869     3.824380    -4.250539     202.98
 H      -3.120109     4.656689    -3.835994      22.22
 C      -2.636533     1.436252    -3.904583      60.82
 H      -2.149141     1.193040    -4.805604      27.60
 C      -3.394231     0.413381    -1.829907      35.67
 C      -3.604735    -0.779529    -0.920740      72.53
 H      -4.348244    -1.465589    -1.611339      26.14
 O      -4.446129    -0.450299     0.264717     130.83
 H      -4.025911    -0.066872     1.031139      23.75
 C      -2.350397    -1.680918    -0.626547      72.72
 H      -1.953376    -1.737100    -1.776856      24.16
 C      -2.665382    -3.163094    -0.064285     112.83
 O      -3.288913    -3.947808    -1.076596     208.91
 H      -2.723224    -3.894855    -1.920298      27.17
 H      -3.444944    -3.033374     0.774961      24.79
 H      -1.650662    -3.378029     0.406173      25.19
 C       2.018735    -1.245351    -0.672734      60.54
 H       2.532482    -2.083600    -1.188228      22.94
 C       1.859290     0.739776     0.559939      30.31
 H       2.249291     1.849798     0.812270      20.42
 C       0.498033     0.331595     0.895684     -23.61
 O      -0.431343     1.211694     1.626207     201.76
 C      -0.552571     2.589552     1.317232     108.99
 H      -0.260302     3.142787     2.230112      24.44
 H       0.417831     3.089290     0.866140      25.11
 H      -1.415357     3.040408     0.509460      23.72
 C      -0.263490    -0.822137     0.217566     -19.65
 O      -1.631283    -0.933073     0.333895     137.59
 C       0.612843    -1.585122    -0.590900      70.87
 H       0.213053    -2.401302    -0.968987      27.12
 C       2.709957    -0.156222    -0.266833      25.67
 C       3.971807     0.351134    -0.844942      93.15
 H       4.042879    -0.110006    -1.975494      23.92
 O       4.062564     1.731245    -1.032157     253.06
 H       4.357088     2.264566    -0.277778      25.06
 C       5.181665    -0.331818    -0.200581      84.87
 H       4.919982    -0.177401     1.033162      24.31
 O       5.015256    -1.738994    -0.336215     287.49
 H       5.105015    -2.007440    -1.336480      27.37
 C       6.622609    -0.023948    -0.708276     120.12
 O       7.106942     1.338167    -0.794846     277.01
 H       7.208924     1.631443     0.169854      28.79
 H       6.834531    -0.362399    -1.647977      31.07
 H       7.255884    -0.507569    -0.040781      29.71
55
name= lig-ACN-Water-frame_480
 C      -2.808046     0.281236    -3.050134      60.71
 H      -2.504463    -0.690201    -3.377915      24.07
 C      -3.827677     1.730156    -1.319238      52.99
 H      -4.099019     1.948150    -0.193631      18.80
 C      -3.736754     2.894385    -2.129025      15.91
 O      -4.202900     4.173836    -1.814058     201.54
 C      -4.962715     4.193111    -0.420647     104.33
 H      -5.903600     3.484254    -0.559472      27.05
 H      -5.597625     5.068857    -0.572680      27.11
 H      -4.253818     4.041966     0.478660      25.52
 C      -3.070433     2.710851    -3.414334      -5.62
 O      -2.779191     3.748181    -4.212226     141.99
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 H      -3.258192     4.645123    -3.921455      23.89
 C      -2.591369     1.399072    -3.839608      55.36
 H      -2.249551     1.503744    -4.907602      22.93
 C      -3.374920     0.472746    -1.687626      38.58
 C      -3.650130    -0.807859    -0.867431      88.53
 H      -4.479409    -1.470332    -1.413484      23.00
 O      -4.346875    -0.441288     0.327513     179.82
 H      -3.628560    -0.285114     0.968843      25.73
 C      -2.399458    -1.708673    -0.596122      83.64
 H      -1.602345    -1.914930    -1.415077      23.37
 C      -2.707807    -3.048282    -0.101430     121.35
 O      -3.286669    -3.932423    -1.142453     138.11
 H      -3.010799    -3.754509    -2.195764      22.89
 H      -3.449092    -3.112254     0.839082      25.32
 H      -1.891385    -3.727905     0.153628      25.92
 C       1.945165    -1.333221    -0.647934      14.08
 H       2.691236    -1.935611    -1.200170      19.02
 C       1.752076     0.671779     0.599394      57.04
 H       2.056181     1.644773     1.027733      22.06
 C       0.442717     0.256783     0.830859      39.99
 O      -0.409716     1.110786     1.641366     177.41
 C      -0.531463     2.614713     1.368073      94.06
 H      -0.831929     3.076981     2.326631      24.74
 H       0.266414     2.903802     0.488997      22.29
 H      -1.647235     2.593699     0.985199      23.58
 C      -0.106452    -0.790949     0.182738      25.47
 O      -1.492152    -0.913495     0.337005     139.88
 C       0.558776    -1.635877    -0.678567      79.97
 H       0.309910    -2.436427    -1.296669      22.88
 C       2.617119    -0.079443    -0.153183     -16.35
 C       3.997529     0.323469    -0.884260      73.74
 H       3.798962    -0.012016    -2.043821      20.61
 O       4.189493     1.801555    -1.033044     213.79
 H       4.349548     2.232273    -0.072043      21.98
 C       5.184775    -0.281110    -0.197175      93.02
 H       5.321749    -0.007943     1.038723      22.80
 O       5.060013    -1.678951    -0.340654     276.46
 H       4.813175    -1.910224    -1.315872      24.76
 C       6.607731    -0.111698    -0.692037     109.02
 O       7.128991     1.337515    -0.799588     258.98
 H       7.029176     1.877614     0.043749      27.55
 H       6.568515    -0.561110    -1.644124      31.20
 H       7.173566    -0.735845    -0.117533      30.99
55
name= lig-ACN-Water-frame_481
 C      -2.819590     0.284356    -2.981854      46.29
 H      -2.312599    -0.589643    -3.273472      23.94
 C      -3.855880     1.759742    -1.213664      50.87
 H      -4.592991     1.653164    -0.339699      21.87
 C      -3.772329     2.870362    -2.091729       7.36
 O      -4.166546     4.157909    -1.720982     233.37
 C      -4.980784     4.192445    -0.538644     103.64
 H      -5.591582     3.179341    -0.410586      24.55
 H      -5.427881     5.157141    -0.530488      23.94
 H      -4.322900     4.216490     0.429481      26.14
 C      -3.078246     2.714363    -3.310202      28.94
 O      -2.776911     3.740260    -4.246802     178.90
 H      -3.071600     4.725123    -3.992328      22.87
 C      -2.639402     1.480349    -3.763460      58.68
 H      -2.082654     1.291983    -4.779805      24.54
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 C      -3.338093     0.465453    -1.700914      45.14
 C      -3.675256    -0.783375    -0.861632      83.88
 H      -4.234299    -1.546594    -1.504563      25.09
 O      -4.284110    -0.507827     0.421385     192.56
 H      -3.685523    -0.037334     1.125298      19.90
 C      -2.321523    -1.615770    -0.603971      73.11
 H      -2.052954    -1.648081    -1.697772      24.39
 C      -2.706703    -3.141045    -0.108768     105.46
 O      -3.385120    -3.892632    -1.135732     166.54
 H      -2.778410    -3.802990    -2.022241      24.99
 H      -3.569675    -2.998396     0.758872      23.35
 H      -1.777824    -3.418599     0.344523      25.75
 C       2.086229    -1.380196    -0.781169      61.30
 H       2.580067    -1.993082    -1.535718      21.48
 C       1.695776     0.726828     0.714934      56.86
 H       2.034835     1.555589     1.215157      22.84
 C       0.369918     0.386361     0.819423     -15.76
 O      -0.409471     1.017951     1.711459     214.26
 C      -0.643048     2.492737     1.400557      87.62
 H      -0.332655     3.096246     2.258902      22.85
 H       0.206825     3.033072     0.652482      22.73
 H      -1.606139     2.595074     0.781835      22.40
 C      -0.185132    -0.824936     0.090865     -20.09
 O      -1.480444    -0.924642     0.368552     149.32
 C       0.724217    -1.677869    -0.685418      57.59
 H       0.159999    -2.499814    -1.280266      22.32
 C       2.491609    -0.180522    -0.234604     -21.06
 C       3.942497     0.443165    -0.831679      68.53
 H       4.069656    -0.034470    -1.968143      22.01
 O       4.237258     1.822616    -1.052255     228.90
 H       4.252738     2.487361    -0.155261      21.03
 C       5.226197    -0.273464    -0.178247      69.55
 H       5.007816     0.095008     1.013876      22.87
 O       5.048472    -1.758511    -0.240218     247.48
 H       5.161373    -2.019339    -1.236435      28.00
 C       6.685684    -0.019776    -0.755303     114.22
 O       7.142336     1.271333    -0.823397     258.29
 H       7.235965     1.568313     0.104505      29.25
 H       6.770419    -0.271226    -1.821765      29.69
 H       7.361893    -0.552119    -0.210696      31.05
55
name= lig-ACN-Water-frame_482
 C      -2.754812     0.386378    -2.877336      82.04
 H      -2.641839    -0.582073    -3.323161      24.65
 C      -3.890689     1.666265    -1.234612      68.51
 H      -4.501892     1.736770    -0.338071      20.67
 C      -3.719297     2.846093    -2.006421      22.19
 O      -4.135314     4.108895    -1.681423     230.72
 C      -4.979092     4.259244    -0.547326     130.30
 H      -5.828573     3.394518    -0.482168      25.35
 H      -5.645454     5.027801    -0.691941      26.50
 H      -4.270862     4.300848     0.373563      25.23
 C      -3.055412     2.770862    -3.318029      26.09
 O      -2.788862     3.766892    -4.261792     185.80
 H      -3.179294     4.622850    -3.949843      23.92
 C      -2.671455     1.481311    -3.703190      45.62
 H      -2.031398     1.511934    -4.711053      25.70
 C      -3.446637     0.458907    -1.646918      50.18
 C      -3.582371    -0.751351    -0.787397     104.65
 H      -4.412615    -1.248762    -1.236557      25.99
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 O      -4.321744    -0.603192     0.479263     150.94
 H      -3.682620    -0.059477     1.122527      24.96
 C      -2.368664    -1.647472    -0.669614     104.32
 H      -1.637274    -1.695516    -1.449765      26.21
 C      -2.672403    -3.066945    -0.106706     111.18
 O      -3.433131    -3.844464    -1.089399     187.47
 H      -2.902645    -4.200541    -1.764021      29.99
 H      -3.442041    -2.921361     0.866765      24.25
 H      -1.933166    -3.755810     0.175107      27.89
 C       2.113074    -1.304952    -0.945114      12.11
 H       2.846427    -1.783599    -1.575883      18.96
 C       1.812880     0.605996     0.616155      77.47
 H       2.273173     1.336814     1.064286      26.55
 C       0.375056     0.298643     0.745115     -29.20
 O      -0.497062     1.051807     1.823180     135.35
 C      -0.688899     2.408145     1.409904     101.08
 H      -0.751842     2.973260     2.390239      24.39
 H       0.171730     2.522292     0.521745      23.35
 H      -1.717814     2.627702     1.123192      24.95
 C      -0.116862    -0.763925     0.065773      -9.18
 O      -1.565211    -1.015380     0.328801     153.77
 C       0.734369    -1.675743    -0.613708      57.29
 H       0.318767    -2.765595    -1.029724      22.37
 C       2.610652    -0.015400    -0.316545      -0.48
 C       3.970732     0.400192    -0.781560      72.94
 H       3.814179     0.070358    -1.975933      21.74
 O       4.169825     1.875230    -1.058225     180.72
 H       4.557416     2.358439    -0.163179      20.69
 C       5.220802    -0.340902    -0.154733      80.03
 H       5.507142    -0.181127     1.049899      23.93
 O       5.050897    -1.783431    -0.085776     266.13
 H       5.135848    -2.128214    -1.022775      28.52
 C       6.680883    -0.037353    -0.834528      99.21
 O       7.210671     1.361531    -0.832960     185.66
 H       7.433911     1.760500     0.042219      26.31
 H       6.620162    -0.525288    -1.865452      29.18
 H       7.252475    -0.718584    -0.328896      31.85
55
name= lig-ACN-Water-frame_483
 C      -2.762450     0.361361    -2.837035      56.37
 H      -2.415296    -0.611483    -3.246960      25.09
 C      -3.983652     1.744680    -1.214585      63.35
 H      -4.182367     1.938860    -0.218424      25.07
 C      -3.630621     2.855987    -2.023442      22.45
 O      -4.107652     4.105166    -1.694870     175.74
 C      -5.048122     4.333334    -0.478949     105.03
 H      -5.782234     3.450482    -0.490895      27.96
 H      -5.353770     5.253100    -0.808121      28.93
 H      -4.653930     4.431364     0.646449      27.60
 C      -3.044253     2.795717    -3.312416       4.25
 O      -2.836306     3.806144    -4.215156     162.43
 H      -3.157735     4.693265    -4.025030      23.07
 C      -2.588054     1.522561    -3.700871      46.31
 H      -2.309685     1.311854    -4.820367      23.75
 C      -3.449128     0.451129    -1.582711      25.13
 C      -3.721384    -0.858750    -0.781227      85.78
 H      -4.207015    -1.551570    -1.353862      27.67
 O      -4.320937    -0.650278     0.535929     154.10
 H      -3.692200    -0.185258     1.190719      25.46
 C      -2.310056    -1.757766    -0.709744      70.18
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 H      -2.072352    -1.902463    -1.709665      27.86
 C      -2.679755    -3.069354    -0.129682     121.90
 O      -3.529277    -3.825379    -1.013477     176.49
 H      -2.984689    -3.933025    -1.799089      30.36
 H      -3.229200    -2.963093     0.960911      24.23
 H      -1.700625    -3.391945     0.073854      27.63
 C       2.013544    -1.095995    -0.974572      62.22
 H       2.488892    -1.885474    -1.547017      25.08
 C       1.822393     0.599669     0.560259      47.31
 H       2.094320     1.360511     1.129336      26.19
 C       0.453009     0.315597     0.878949      -9.01
 O      -0.383158     0.934579     1.751959     198.42
 C      -0.770288     2.424248     1.446603      92.40
 H      -0.524763     3.133766     2.296495      25.57
 H      -0.057518     3.006258     0.640212      25.91
 H      -1.731679     2.311380     0.895419      25.16
 C      -0.198871    -0.829425     0.118585     -13.20
 O      -1.454353    -1.052074     0.331553     125.18
 C       0.792569    -1.612406    -0.612938      55.64
 H       0.522814    -2.817075    -0.945902      24.33
 C       2.651699    -0.057295    -0.440230      32.13
 C       4.108959     0.392484    -0.851570      87.88
 H       4.425408    -0.105808    -1.944288      24.19
 O       4.081131     1.853009    -1.007723     213.43
 H       4.401547     2.411635    -0.239644      23.11
 C       5.315154    -0.348527    -0.101409      84.98
 H       5.257306     0.255285     0.960516      24.88
 O       5.066037    -1.790654     0.024641     267.91
 H       4.832378    -2.101002    -0.872543      28.74
 C       6.619228    -0.091329    -0.850963      90.60
 O       7.240797     1.390037    -0.884390     165.30
 H       7.083836     1.687557     0.064598      28.11
 H       6.528037    -0.122200    -2.025102      25.21
 H       7.431818    -0.626805    -0.466673      29.70
55
name= lig-ACN-Water-frame_484
 C      -2.819175     0.374452    -2.827919      56.39
 H      -2.339121    -0.611426    -3.111353      23.91
 C      -3.895684     1.767833    -1.170928      52.60
 H      -4.485191     1.875510    -0.325950      21.63
 C      -3.680541     2.915042    -1.995200      25.20
 O      -4.105798     4.195793    -1.607596     230.12
 C      -5.070279     4.405925    -0.548946     115.35
 H      -5.996875     3.774428    -0.485686      28.22
 H      -5.513616     5.399518    -0.577503      26.75
 H      -4.290756     4.299288     0.328567      24.73
 C      -2.991648     2.740569    -3.309612       0.39
 O      -2.876846     3.840474    -4.189034     153.85
 H      -3.127004     4.670689    -3.779187      28.50
 C      -2.551175     1.456493    -3.670263      62.85
 H      -2.104689     1.300816    -4.697882      24.31
 C      -3.456127     0.460830    -1.588422      30.27
 C      -3.721916    -0.944131    -0.796072      76.13
 H      -4.484269    -1.403354    -1.193443      26.22
 O      -4.321158    -0.713682     0.532475     167.08
 H      -3.714188    -0.246026     1.085013      28.95
 C      -2.406088    -1.691723    -0.669697      93.98
 H      -1.791670    -1.670370    -1.472257      26.83
 C      -2.601260    -3.172823    -0.080920     114.89
 O      -3.582299    -3.833075    -0.949867     117.70
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 H      -3.385768    -3.728901    -1.998182      26.60
 H      -3.217999    -3.040799     0.917321      25.33
 H      -1.839127    -3.895749     0.029858      28.18
 C       1.993117    -1.182896    -1.056216      36.96
 H       2.544329    -1.594930    -1.916096      21.24
 C       1.847410     0.724345     0.581763      49.90
 H       2.276518     1.556874     1.039786      22.41
 C       0.545780     0.199136     0.820355      36.49
 O      -0.222769     0.950654     1.710974     161.76
 C      -0.798852     2.442157     1.401733      83.96
 H      -0.910862     2.647856     2.522468      24.55
 H      -0.017328     2.752614     0.585196      23.80
 H      -1.793617     2.374992     1.096496      26.83
 C      -0.021320    -0.843265     0.224310      27.36
 O      -1.461561    -1.116683     0.298301     162.23
 C       0.699358    -1.563899    -0.638042      65.92
 H       0.151411    -2.495247    -1.310009      21.86
 C       2.648656     0.001015    -0.404026     -48.27
 C       4.158312     0.366045    -0.921581      78.28
 H       4.196894     0.175760    -2.153681      23.20
 O       4.048175     1.809287    -0.969126     249.87
 H       4.164969     2.140357    -0.122309      24.34
 C       5.336939    -0.226023    -0.051202      83.59
 H       5.456199    -0.031539     1.100295      24.90
 O       5.089645    -1.723985     0.108877     249.67
 H       4.937082    -2.091077    -0.810687      28.47
 C       6.704228     0.010199    -0.890949      94.08
 O       7.132473     1.300522    -0.871709     232.07
 H       7.375038     1.718722     0.034632      25.02
 H       6.344735    -0.389485    -1.993012      26.95
 H       7.416704    -0.824379    -0.650122      29.01
55
name= lig-ACN-Water-frame_485
 C      -2.812163     0.317805    -2.822708      56.43
 H      -2.682915    -0.724902    -3.271678      22.78
 C      -3.833992     1.750422    -1.137512      62.89
 H      -4.571963     1.747130    -0.370856      21.62
 C      -3.728124     2.919894    -1.975702      21.47
 O      -4.093888     4.278603    -1.645866     253.65
 C      -5.033099     4.469040    -0.551851     120.91
 H      -5.802711     3.777030    -0.740285      25.54
 H      -5.272492     5.546690    -0.706879      24.08
 H      -4.785271     4.202534     0.624011      24.71
 C      -3.023632     2.796118    -3.209279      19.55
 O      -2.876478     3.768763    -4.146043     227.57
 H      -3.308590     4.617153    -3.944433      24.12
 C      -2.560744     1.463583    -3.646364      50.55
 H      -1.839976     1.417195    -4.436541      27.09
 C      -3.490156     0.453691    -1.566759      37.66
 C      -3.696416    -0.797944    -0.769105      92.61
 H      -4.130142    -1.415605    -1.361790      28.68
 O      -4.322458    -0.764522     0.506493     212.38
 H      -3.725360    -0.414507     1.191995      25.47
 C      -2.290613    -1.800166    -0.593678      73.77
 H      -2.052686    -1.898752    -1.581540      28.12
 C      -2.620988    -3.235670    -0.120173     113.69
 O      -3.667050    -3.876819    -0.917603     122.78
 H      -3.244198    -3.714839    -1.871919      28.24
 H      -2.961029    -3.217933     0.941179      27.13
 H      -1.613962    -3.667577    -0.146427      27.20
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 C       2.068145    -1.177673    -1.067699      49.93
 H       2.549598    -1.604322    -1.955176      24.63
 C       1.976180     0.692079     0.491600      55.90
 H       2.225492     1.679891     0.968586      21.78
 C       0.617580     0.348749     0.845008     -44.81
 O      -0.174520     1.050575     1.758558     235.62
 C      -0.774113     2.286785     1.388295     123.21
 H      -0.827534     3.015754     2.260352      24.75
 H      -0.030420     3.112764     0.989951      24.26
 H      -1.532472     2.246108     0.738067      28.84
 C      -0.081567    -0.949078     0.197366     -47.55
 O      -1.466579    -1.061815     0.423566      99.56
 C       0.715298    -1.645736    -0.873230      48.34
 H       0.034113    -2.312353    -1.640296      21.62
 C       2.645243    -0.100788    -0.409396      54.96
 C       3.951318     0.395165    -0.830217      78.30
 H       4.163314    -0.217437    -1.904031      25.04
 O       4.092257     1.843156    -0.928165     194.73
 H       4.486536     2.320951    -0.125567      22.69
 C       5.348252    -0.250207    -0.119828      81.18
 H       5.419980     0.463765     0.778010      26.04
 O       5.132168    -1.596606     0.149178     250.13
 H       5.207029    -2.060594    -0.749142      29.55
 C       6.646717    -0.100129    -0.871254      87.37
 O       7.068521     1.337240    -0.856729     178.57
 H       7.282313     1.508020     0.100137      28.81
 H       6.540224    -0.200966    -2.109878      26.39
 H       7.528144    -0.663181    -0.360555      28.05
55
name= lig-ACN-Water-frame_486
 C      -2.845788     0.317265    -2.856508      56.33
 H      -2.563124    -0.661365    -3.320801      25.07
 C      -3.919759     1.786116    -1.109652      60.94
 H      -4.095330     1.948679    -0.017204      20.30
 C      -3.711990     2.944337    -1.919956      24.85
 O      -4.035229     4.246635    -1.683985     250.62
 C      -5.058756     4.506979    -0.589654      95.19
 H      -5.986467     4.124993    -0.814709      30.91
 H      -5.251769     5.709985    -0.534275      26.02
 H      -4.510497     4.163276     0.409115      27.09
 C      -3.068849     2.723620    -3.141080       8.23
 O      -2.858544     3.734766    -4.130236     168.47
 H      -3.305214     4.616659    -3.795486      23.67
 C      -2.573134     1.525025    -3.510622      64.63
 H      -2.245515     1.478703    -4.494469      25.67
 C      -3.421454     0.483614    -1.579226      26.02
 C      -3.553499    -0.878542    -0.737890      99.26
 H      -4.224104    -1.359378    -1.225950      28.08
 O      -4.362872    -0.770399     0.494775     169.94
 H      -3.769727    -0.421496     1.279436      25.67
 C      -2.319593    -1.738816    -0.535833      81.61
 H      -1.587224    -1.747825    -1.283501      26.29
 C      -2.613575    -3.255941    -0.101206     115.50
 O      -3.675776    -3.901267    -0.931254     174.16
 H      -3.349382    -4.180979    -1.729011      33.36
 H      -2.909229    -3.447656     0.877655      28.49
 H      -1.776582    -3.941532    -0.362541      26.84
 C       2.031438    -1.239568    -1.128519      42.08
 H       2.695794    -1.855649    -1.739794      23.56
 C       1.842486     0.623469     0.522081      40.66
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 H       2.582528     1.516986     0.777310      18.58
 C       0.555759     0.295704     0.787514       8.30
 O      -0.109439     1.070919     1.857825     196.62
 C      -0.685385     2.336006     1.316652     113.67
 H      -1.396499     2.590202     2.116928      25.45
 H       0.113552     2.827560     0.714121      25.18
 H      -1.355080     2.071678     0.642151      29.25
 C      -0.022043    -0.871614     0.068299     -12.40
 O      -1.379965    -1.053807     0.498196     127.07
 C       0.681550    -1.548759    -0.926992      75.79
 H       0.507952    -2.455904    -1.581826      22.68
 C       2.657054    -0.186157    -0.394829     -10.74
 C       4.054290     0.382532    -0.826670      90.64
 H       3.997217     0.352990    -2.081733      21.13
 O       4.119439     1.882042    -0.920572     149.39
 H       4.684131     2.282912    -0.074169      19.11
 C       5.224669    -0.165982    -0.188159     101.40
 H       5.405486     0.229915     0.857393      24.53
 O       5.168503    -1.568499     0.213946     238.06
 H       5.131544    -2.127366    -0.593753      29.28
 C       6.607769    -0.050314    -0.894262      80.33
 O       7.032994     1.368982    -0.856965     163.35
 H       6.951802     1.819321     0.010925      25.90
 H       6.732594    -0.582435    -2.016594      23.54
 H       7.321964    -0.792630    -0.228327      26.51
55
name= lig-ACN-Water-frame_487
 C      -2.874316     0.366830    -2.784647      58.90
 H      -2.469031    -0.591379    -3.080579      23.77
 C      -3.883761     1.752361    -1.064315      64.12
 H      -4.185563     1.866542     0.071151      20.27
 C      -3.698365     2.903488    -1.859656      21.12
 O      -4.062204     4.248042    -1.638733     252.55
 C      -5.010440     4.564757    -0.680206     117.62
 H      -5.904052     4.083805    -0.801691      30.38
 H      -4.952117     5.770422    -0.586750      25.81
 H      -4.699443     4.103240     0.416022      26.52
 C      -3.077911     2.784447    -3.175467      -1.59
 O      -2.864873     3.743035    -4.072499     156.42
 H      -3.176096     4.738816    -3.799112      22.02
 C      -2.579469     1.461948    -3.587404      53.11
 H      -2.211911     1.408797    -4.567692      24.68
 C      -3.386996     0.464648    -1.469725      36.71
 C      -3.595297    -0.900522    -0.719997      96.41
 H      -3.967692    -1.566303    -1.337367      29.10
 O      -4.358447    -0.740175     0.511789     211.38
 H      -3.781896    -0.340532     1.222456      26.31
 C      -2.224381    -1.713402    -0.458811      95.09
 H      -1.992547    -1.679685    -1.569167      24.35
 C      -2.594670    -3.294110    -0.129127     112.41
 O      -3.684830    -3.906909    -0.937859     191.98
 H      -3.166830    -4.173787    -1.737766      29.83
 H      -2.912187    -3.223084     0.794587      29.64
 H      -1.577063    -3.832509    -0.084855      26.64
 C       2.082833    -1.274051    -1.122437      46.29
 H       2.618822    -1.948919    -1.791055      23.13
 C       1.878956     0.518339     0.476332      39.40
 H       2.013422     1.418741     1.283748      19.60
 C       0.505444     0.255693     0.831651      14.80
 O      -0.022709     0.975916     1.869659     191.03
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 C      -0.683548     2.312490     1.171463      89.45
 H      -1.197975     2.839400     1.981788      25.55
 H       0.055940     3.148307     1.175348      24.75
 H      -1.111563     2.078492     0.335584      27.99
 C      -0.126060    -0.681374     0.026452      -1.91
 O      -1.308357    -1.130121     0.511644     196.48
 C       0.669980    -1.507654    -0.908246      46.84
 H       0.058799    -2.311264    -1.042060      18.84
 C       2.646033    -0.134197    -0.425388      25.14
 C       4.032238     0.461107    -0.990618      73.34
 H       4.257209    -0.127254    -2.117226      22.80
 O       4.127219     1.886952    -0.887949     212.36
 H       4.293434     2.326636     0.100168      19.13
 C       5.283785    -0.191241    -0.124841      80.46
 H       5.229125     0.458412     0.789533      26.73
 O       5.142888    -1.620202     0.253251     243.74
 H       4.900421    -2.056471    -0.579182      30.08
 C       6.592105     0.074243    -0.816324      87.59
 O       7.001787     1.379243    -0.952608     197.86
 H       7.235481     1.655469    -0.040454      28.92
 H       6.461798    -0.276221    -1.972658      27.61
 H       7.464523    -0.561181    -0.161990      27.32
55
name= lig-ACN-Water-frame_488
 C      -2.797847     0.365263    -2.689961      53.54
 H      -2.636173    -0.603085    -3.091669      24.30
 C      -3.787161     1.736964    -0.954045      55.67
 H      -4.676898     1.825155    -0.170571      20.31
 C      -3.668488     2.855875    -1.906592       1.06
 O      -4.026792     4.213182    -1.643823     207.78
 C      -5.007447     4.586017    -0.617271     119.22
 H      -5.912465     4.426680    -1.059356      26.74
 H      -5.109392     5.841792    -0.674600      24.92
 H      -4.812408     4.192503     0.447551      25.47
 C      -3.044849     2.707945    -3.176505      11.92
 O      -2.864377     3.860067    -4.055046     200.96
 H      -3.375244     4.674960    -3.672530      21.17
 C      -2.680265     1.461488    -3.651429      62.07
 H      -1.959218     1.281736    -4.429039      24.25
 C      -3.418243     0.433069    -1.405765      23.09
 C      -3.614453    -0.859054    -0.648474      99.21
 H      -4.318522    -1.382127    -1.166365      26.19
 O      -4.369376    -0.713936     0.535903     215.11
 H      -3.841929    -0.302332     1.200050      27.92
 C      -2.255572    -1.799930    -0.534333      88.87
 H      -1.512188    -1.817588    -1.463921      22.00
 C      -2.582945    -3.190006    -0.055827     121.59
 O      -3.579088    -3.890724    -0.935365     141.58
 H      -3.281218    -3.869623    -1.991007      27.17
 H      -3.027532    -3.278943     0.808041      29.45
 H      -1.679059    -3.906756    -0.118720      25.86
 C       2.011222    -1.230510    -1.066201      52.87
 H       2.479007    -1.810416    -1.858940      23.04
 C       1.946608     0.537680     0.551493      37.77
 H       2.691862     1.319224     1.051430      20.38
 C       0.600319     0.259271     0.820668      10.00
 O      -0.077065     0.999818     1.803707     251.46
 C      -0.589743     2.275405     1.196226      99.50
 H      -1.495098     2.458660     1.712898      26.18
 H       0.321356     2.783754     1.015995      26.15
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 H      -0.947642     2.093819     0.251183      29.17
 C      -0.139714    -0.667792     0.010796       1.36
 O      -1.380143    -1.239011     0.478496     198.70
 C       0.649095    -1.489269    -0.781499      70.49
 H       0.409206    -2.227621    -1.347832      24.29
 C       2.665538    -0.093492    -0.613887      12.01
 C       4.017542     0.390013    -0.920786      77.01
 H       4.185557     0.407112    -2.208232      22.35
 O       4.101062     1.875311    -0.899418     201.25
 H       4.267793     2.141979     0.024016      26.82
 C       5.236791    -0.188442    -0.014347      92.25
 H       5.206889     0.242667     0.978152      28.17
 O       5.100733    -1.608665     0.237030     245.88
 H       4.937399    -2.049898    -0.656691      28.93
 C       6.609331     0.040731    -0.777620      84.39
 O       7.005449     1.500688    -1.037258     102.98
 H       7.316107     1.945089    -0.172475      25.32
 H       6.503547    -0.459235    -1.847515      28.66
 H       7.636482    -0.591578    -0.402041      28.09
55
name= lig-ACN-Water-frame_489
 C      -2.763920     0.320885    -2.688275      69.32
 H      -2.412383    -0.616874    -3.031017      22.92
 C      -3.814572     1.790919    -0.999663      52.98
 H      -4.339414     1.947329     0.043326      19.56
 C      -3.649400     2.839535    -1.873546      26.73
 O      -3.963221     4.146390    -1.621952     206.86
 C      -5.064101     4.618204    -0.643273     103.83
 H      -6.031769     4.230099    -0.802145      27.16
 H      -4.683245     5.767984    -0.509919      24.43
 H      -4.836853     4.157979     0.371683      25.77
 C      -3.040989     2.761863    -3.215949      -3.39
 O      -2.871918     3.896016    -3.993010     113.94
 H      -3.380289     4.626395    -3.644632      27.80
 C      -2.682632     1.392468    -3.552491      35.13
 H      -2.439906     1.298173    -4.657226      23.12
 C      -3.356119     0.493175    -1.428327      31.09
 C      -3.628153    -0.887623    -0.682975      82.40
 H      -4.260595    -1.405417    -1.324702      26.75
 O      -4.377235    -0.688731     0.634051     207.77
 H      -3.860110    -0.156072     1.316572      24.20
 C      -2.371533    -1.795741    -0.581592      67.69
 H      -1.931547    -1.909052    -1.728722      21.86
 C      -2.623236    -3.225170    -0.017230     115.74
 O      -3.489835    -3.858416    -0.943351     200.47
 H      -3.023058    -3.629194    -1.847945      28.03
 H      -2.977430    -3.053506     0.939343      27.20
 H      -1.569134    -3.687820     0.122088      25.47
 C       1.947118    -1.157803    -1.167212      52.93
 H       2.483208    -1.771177    -1.904222      23.75
 C       2.096751     0.584168     0.506804      40.90
 H       2.560301     1.381653     1.133840      20.65
 C       0.630585     0.280872     0.804568     -42.91
 O      -0.161455     0.989896     1.758607     227.94
 C      -0.504149     2.243141     1.147807     122.64
 H      -1.258085     2.653738     1.791834      26.83
 H       0.117883     3.061190     1.322370      26.61
 H      -0.754049     2.030234     0.202748      29.64
 C      -0.096592    -0.833099     0.174729      -8.45
 O      -1.420754    -1.214255     0.460891     128.97
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 C       0.674282    -1.574091    -0.796138      56.37
 H       0.172701    -2.270908    -1.239250      23.88
 C       2.614769    -0.028135    -0.523401      27.68
 C       4.099025     0.415319    -0.852441      75.59
 H       4.418464    -0.266721    -1.944295      24.26
 O       4.062947     1.851351    -0.867599     186.33
 H       4.459812     2.313360    -0.189401      25.82
 C       5.197628    -0.184948     0.012554      94.80
 H       5.246932     0.253759     0.947155      29.17
 O       5.055899    -1.607684     0.179136     254.23
 H       5.143991    -2.023090    -0.745319      29.08
 C       6.655647     0.095350    -0.812544      69.33
 O       6.998652     1.525276    -1.091658     160.20
 H       6.916914     1.839338    -0.112312      26.95
 H       6.530539    -0.386805    -1.794015      29.99
 H       7.403385    -0.406966     0.081333      26.78
55
name= lig-ACN-Water-frame_490
 C      -2.767313     0.323210    -2.704991      47.19
 H      -2.406437    -0.648468    -3.035719      25.06
 C      -3.832579     1.744209    -1.069074      63.80
 H      -3.950836     1.942411     0.020486      21.06
 C      -3.627997     2.900414    -1.890276      16.87
 O      -3.988938     4.205748    -1.543975     264.12
 C      -4.963773     4.522562    -0.639422     115.34
 H      -5.894482     4.482142    -1.180918      27.33
 H      -5.050275     5.776165    -0.597601      26.13
 H      -4.825130     4.080229     0.324235      30.93
 C      -3.079628     2.726870    -3.131780      13.08
 O      -2.876375     3.847678    -3.946207     176.32
 H      -3.357931     4.580870    -3.581484      24.62
 C      -2.643617     1.479708    -3.583890      61.62
 H      -2.332353     1.163076    -4.659068      23.50
 C      -3.297546     0.454214    -1.393275      29.07
 C      -3.679588    -0.808421    -0.616222      91.17
 H      -4.332423    -1.414282    -1.158684      26.11
 O      -4.370060    -0.705240     0.612692     212.14
 H      -3.728847    -0.200739     1.307760      22.28
 C      -2.408816    -1.738105    -0.484438      62.37
 H      -1.982513    -1.762218    -1.627089      22.44
 C      -2.623477    -3.151248     0.028698     115.23
 O      -3.461585    -3.888793    -0.953060     208.97
 H      -2.966425    -4.088008    -1.716549      31.98
 H      -3.358248    -3.249155     0.863901      24.70
 H      -1.676085    -3.747978     0.205986      25.56
 C       1.989857    -1.089975    -1.271305      31.88
 H       2.527101    -1.574516    -2.122126      24.72
 C       1.859015     0.661019     0.610094      39.35
 H       2.203698     1.493071     1.107378      21.49
 C       0.605357     0.193172     0.859371      23.76
 O      -0.166874     0.944354     1.708208     222.38
 C      -0.500861     2.357348     1.144770     108.94
 H      -1.413159     2.659731     1.618576      26.29
 H       0.405019     2.792065     1.228642      26.97
 H      -0.721786     2.465124     0.168839      28.52
 C       0.029740    -0.990710     0.274299       4.47
 O      -1.406946    -1.086047     0.445698     127.35
 C       0.627866    -1.635506    -0.811056      61.14
 H       0.276300    -2.513008    -1.216538      23.56
 C       2.707074    -0.107081    -0.489764     -13.69
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 C       4.066096     0.364195    -0.821038      80.30
 H       4.261688     0.264785    -2.126075      19.49
 O       4.062357     1.844338    -0.913990     240.77
 H       4.332047     2.198153     0.001589      21.17
 C       5.301518    -0.143665    -0.040519     108.64
 H       5.289046     0.218181     0.902996      28.98
 O       5.044941    -1.607614     0.103576     273.87
 H       5.091531    -2.002091    -0.804338      28.66
 C       6.599829     0.157230    -0.734227     108.76
 O       6.952483     1.479224    -1.059384     188.99
 H       7.159053     1.988000    -0.223699      27.03
 H       6.819343    -0.407594    -1.591591      31.09
 H       7.634886    -0.249787    -0.105006      26.84
55
name= lig-ACN-Water-frame_491
 C      -2.762583     0.368568    -2.735506      72.43
 H      -2.573301    -0.608875    -3.232790      22.43
 C      -3.759952     1.734583    -1.000712      62.06
 H      -4.439732     1.798148    -0.183131      21.80
 C      -3.678404     2.887547    -1.817487      25.20
 O      -3.875188     4.252171    -1.544372     253.87
 C      -5.043228     4.507120    -0.603964     108.80
 H      -6.001897     4.048614    -0.928240      25.09
 H      -4.806451     5.670820    -0.356011      24.79
 H      -5.006606     3.952647     0.317999      26.58
 C      -3.060072     2.730337    -3.152250       7.65
 O      -2.881293     3.803994    -3.941972     154.81
 H      -3.381700     4.643472    -3.586156      22.37
 C      -2.618844     1.462899    -3.574975      61.60
 H      -1.891231     1.619318    -4.445258      23.88
 C      -3.351148     0.465696    -1.453886      36.25
 C      -3.619327    -0.829133    -0.585212      95.57
 H      -4.269642    -1.306940    -1.254825      24.67
 O      -4.409032    -0.682303     0.613015     193.23
 H      -3.876558    -0.353574     1.458553      21.95
 C      -2.309499    -1.667141    -0.372016      86.71
 H      -1.663854    -1.840249    -1.341012      21.55
 C      -2.721156    -3.131042     0.053957     101.44
 O      -3.470696    -3.965138    -0.941180     231.65
 H      -2.884669    -4.017158    -1.692241      30.42
 H      -3.231264    -3.038192     1.135112      23.63
 H      -1.753728    -3.609117     0.287860      25.83
 C       1.963530    -1.099844    -1.186467      47.08
 H       2.427215    -1.410348    -2.157226      23.07
 C       1.823441     0.527596     0.520831      59.30
 H       2.155798     1.376534     0.876249      22.11
 C       0.541655     0.074229     0.917142      -9.66
 O      -0.301630     0.991126     1.672135     191.96
 C      -0.452074     2.390707     1.153753     112.60
 H      -1.187075     2.841849     1.849413      25.25
 H       0.332539     3.031229     1.442509      26.20
 H      -0.662156     2.238359     0.197420      28.74
 C      -0.042990    -1.052831     0.203389     -21.01
 O      -1.375148    -0.950141     0.486446     145.53
 C       0.821356    -1.637972    -0.845938      74.09
 H       0.354456    -2.379353    -1.547977      22.88
 C       2.564322    -0.117388    -0.358395      26.41
 C       4.038658     0.458014    -0.903334      61.65
 H       4.101623    -0.166695    -2.068481      22.01
 O       4.061999     1.860823    -0.937132     238.59
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 H       4.180363     2.328062     0.023095      19.25
 C       5.263385    -0.178759    -0.072079     101.68
 H       5.230364     0.177953     0.872605      28.40
 O       5.104580    -1.585800     0.034343     298.24
 H       5.052674    -1.971892    -0.867074      28.72
 C       6.708811     0.071568    -0.702276      87.97
 O       6.930090     1.529472    -1.029275     202.04
 H       7.102141     1.874522    -0.107386      26.50
 H       6.642293    -0.401310    -1.576582      32.56
 H       7.428293    -0.454518     0.200706      27.95
55
name= lig-ACN-Water-frame_492
 C      -2.777349     0.336933    -2.775228      47.63
 H      -2.389116    -0.695747    -3.026963      24.68
 C      -3.802804     1.780346    -0.916220      52.12
 H      -4.393791     1.711097    -0.065585      22.21
 C      -3.625625     2.877831    -1.836493      17.77
 O      -3.841798     4.221293    -1.472989     241.67
 C      -5.063002     4.447821    -0.539217     102.98
 H      -6.006486     4.341106    -1.136585      25.39
 H      -5.216187     5.623458    -0.320757      25.73
 H      -4.710767     3.959421     0.338868      26.34
 C      -3.066580     2.762937    -3.086300      10.14
 O      -2.881202     3.828302    -3.989387     136.45
 H      -3.360034     4.707562    -3.586813      22.67
 C      -2.542785     1.519003    -3.540865      46.62
 H      -2.178223     1.348855    -4.589787      22.65
 C      -3.409655     0.480598    -1.488162      18.30
 C      -3.543374    -0.831547    -0.697869      74.83
 H      -3.984306    -1.668876    -1.168831      26.55
 O      -4.468801    -0.649886     0.620151     125.88
 H      -3.823694    -0.170774     1.220119      27.04
 C      -2.301911    -1.686076    -0.392108      79.75
 H      -1.917996    -1.700153    -1.467900      25.44
 C      -2.714530    -3.158681     0.138998     101.90
 O      -3.461233    -3.962156    -0.842291     153.35
 H      -3.087912    -3.756396    -1.809777      27.22
 H      -3.602677    -3.066308     1.022701      22.48
 H      -1.849171    -3.739553     0.423084      27.00
 C       2.103927    -1.148490    -1.112300      16.21
 H       2.645691    -1.583598    -2.000649      22.03
 C       1.819365     0.495041     0.612833      45.37
 H       2.089498     1.332209     1.113448      23.58
 C       0.486239     0.109009     0.906987       8.21
 O      -0.419707     0.975346     1.660732     197.15
 C      -0.400182     2.349887     1.203817     108.45
 H      -1.336888     2.800181     1.644941      25.93
 H       0.602650     2.775484     1.254739      26.04
 H      -0.634325     2.579639     0.269020      31.65
 C      -0.047634    -0.918538     0.165304      -5.64
 O      -1.431472    -0.976340     0.517604     139.71
 C       0.652859    -1.695599    -0.793010      49.19
 H       0.165068    -2.366191    -1.675743      20.90
 C       2.675653    -0.089100    -0.481319      39.49
 C       3.944227     0.420758    -0.859992      86.71
 H       4.129432     0.250529    -2.141624      23.42
 O       4.038821     1.903925    -0.987963     167.56
 H       4.511270     2.167402    -0.078236      23.05
 C       5.190273    -0.167650    -0.118847     102.09
 H       5.152022     0.204376     0.836947      29.31
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 O       5.152598    -1.621545     0.003449     262.14
 H       5.305346    -1.963143    -0.921039      28.49
 C       6.657763     0.063758    -0.736231      97.23
 O       6.963715     1.476782    -0.963592     245.34
 H       7.053306     1.847134    -0.030768      25.70
 H       6.963275    -0.401787    -1.547129      31.66
 H       7.627149    -0.298669    -0.007428      27.68
55
name= lig-ACN-Water-frame_493
 C      -2.804275     0.385826    -2.704805      61.36
 H      -2.408188    -0.554904    -3.188128      26.60
 C      -3.852633     1.716459    -1.022436      66.18
 H      -3.950085     2.007331    -0.012005      23.60
 C      -3.577359     2.930272    -1.735275       5.70
 O      -3.908732     4.206281    -1.346551     247.55
 C      -4.986717     4.417233    -0.528807     113.54
 H      -5.905585     3.888949    -1.017766      26.27
 H      -4.864233     5.571453    -0.426315      25.76
 H      -5.234008     3.885655     0.380865      28.28
 C      -2.977808     2.778278    -3.133670      -5.64
 O      -2.901497     3.868665    -4.000284     121.24
 H      -3.415783     4.682181    -3.647405      24.26
 C      -2.546477     1.512672    -3.541844      62.94
 H      -2.341392     1.430776    -4.590816      24.50
 C      -3.425603     0.448035    -1.477213      38.24
 C      -3.690644    -0.867667    -0.662530     100.64
 H      -4.452932    -1.215101    -1.297867      25.38
 O      -4.419652    -0.619063     0.479840     190.32
 H      -3.941158    -0.300503     1.253283      25.06
 C      -2.370428    -1.755206    -0.435180      94.77
 H      -1.756743    -2.041642    -1.286746      26.15
 C      -2.704664    -3.139498     0.193725     104.22
 O      -3.484580    -3.923024    -0.737526     147.43
 H      -2.925580    -3.944122    -1.712512      24.45
 H      -3.446395    -2.902616     1.226722      23.53
 H      -1.840198    -3.614233     0.633707      26.47
 C       1.990650    -1.342048    -1.056110      46.59
 H       2.589291    -1.995313    -1.722975      22.72
 C       1.898567     0.570398     0.705502      64.67
 H       2.473393     1.316353     1.270428      22.07
 C       0.531492     0.267062     0.844935     -14.14
 O      -0.432032     0.885395     1.623155     200.38
 C      -0.407846     2.365954     1.191303      99.10
 H      -0.948055     2.970282     2.019803      24.41
 H       0.630733     2.695872     1.617975      22.55
 H      -0.533635     2.292219     0.255231      31.71
 C      -0.162763    -0.851138     0.137157       0.81
 O      -1.461426    -1.116541     0.479324     159.24
 C       0.665517    -1.573757    -0.769892      54.92
 H       0.073924    -2.635410    -1.125919      21.81
 C       2.548406    -0.088325    -0.415852     -33.01
 C       4.035736     0.454282    -0.977104      59.20
 H       4.047330    -0.071273    -2.155906      22.66
 O       4.035657     1.908998    -1.029390     189.96
 H       4.068039     2.315900     0.029560      21.00
 C       5.241336    -0.199975    -0.166877      94.35
 H       5.211769     0.162668     0.822476      28.56
 O       5.165951    -1.657369     0.007820     266.55
 H       5.218336    -2.061958    -0.920580      28.06
 C       6.588119     0.112368    -0.766393     109.11
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 O       7.015434     1.448299    -0.937592     190.44
 H       7.395305     1.814751    -0.076586      26.46
 H       6.568786    -0.350234    -1.633783      33.89
 H       7.160426    -0.487021     0.155204      28.60
55
name= lig-ACN-Water-frame_494
 C      -2.768780     0.391098    -2.741381      54.92
 H      -2.682065    -0.649487    -3.116426      21.80
 C      -3.794585     1.766106    -1.049987      47.40
 H      -4.335764     1.692372    -0.079367      19.87
 C      -3.504686     2.874541    -1.821897      23.13
 O      -3.822542     4.149634    -1.273038     240.77
 C      -5.100018     4.380544    -0.454467     104.85
 H      -6.022347     4.180175    -1.090991      24.98
 H      -5.311648     5.504672    -0.295644      26.00
 H      -4.734670     4.014054     0.521029      24.49
 C      -2.967004     2.871323    -3.067390      28.34
 O      -2.919674     3.900824    -3.981763     213.44
 H      -3.467563     4.623362    -3.676500      24.87
 C      -2.638268     1.541943    -3.556042      48.33
 H      -2.030678     1.460088    -4.395172      26.16
 C      -3.393723     0.438397    -1.444104      22.72
 C      -3.779860    -0.859502    -0.790373      90.24
 H      -4.319162    -1.606665    -1.357939      25.89
 O      -4.432609    -0.594211     0.482680     202.43
 H      -3.687870    -0.348447     1.100785      24.48
 C      -2.442559    -1.874088    -0.501454      82.55
 H      -2.169279    -1.946177    -1.521663      25.84
 C      -2.740671    -3.092955     0.268043     110.31
 O      -3.517731    -3.924562    -0.631226     177.60
 H      -2.875006    -4.152811    -1.385529      28.32
 H      -3.389519    -2.909588     1.363437      23.38
 H      -1.794101    -3.584383     0.429079      25.92
 C       1.934631    -1.272612    -0.912721      44.60
 H       2.479186    -1.984439    -1.516044      22.25
 C       1.903003     0.542767     0.600047      31.82
 H       2.404187     1.408225     1.324753      16.82
 C       0.458380     0.263539     0.762566     -13.74
 O      -0.383264     0.959610     1.634564     234.86
 C      -0.354423     2.332537     1.301903     115.21
 H      -1.332443     2.804174     1.682645      24.03
 H       0.706357     2.908888     1.194292      22.65
 H      -0.659620     2.593703     0.431627      29.30
 C      -0.135630    -0.749906     0.091772       9.83
 O      -1.463229    -1.195264     0.459018     150.39
 C       0.551985    -1.610569    -0.693616      43.55
 H       0.302634    -2.798342    -1.032565      15.95
 C       2.571154    -0.183445    -0.385724      24.44
 C       3.965844     0.362951    -0.990591      79.09
 H       4.185518     0.161128    -2.212289      19.63
 O       4.022664     1.861072    -1.060460     190.14
 H       4.202495     2.160242     0.015096      19.67
 C       5.159935    -0.182976    -0.148833      97.98
 H       5.079693     0.226647     0.877518      26.03
 O       5.145792    -1.651025     0.001277     282.98
 H       5.126434    -1.985080    -0.968297      26.13
 C       6.598738     0.040420    -0.791355     101.79
 O       7.115374     1.481766    -0.944803     222.41
 H       7.144514     1.749083     0.067875      27.52
 H       6.582926    -0.221353    -1.769967      31.36
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 H       7.568485    -0.575541    -0.464019      28.31
55
name= lig-ACN-Water-frame_495
 C      -2.788124     0.373627    -2.809288      62.87
 H      -2.390653    -0.482846    -3.328787      24.65
 C      -3.732839     1.673711    -0.972582      55.74
 H      -4.600104     1.876274    -0.280128      19.32
 C      -3.563385     2.927348    -1.739718      25.04
 O      -3.779412     4.180139    -1.224884     178.27
 C      -5.103628     4.358604    -0.402421     101.97
 H      -5.934862     3.665443    -0.821296      24.21
 H      -5.067762     5.455897    -0.401930      25.76
 H      -5.223079     3.754642     0.566613      23.59
 C      -2.986964     2.826173    -3.110239       9.07
 O      -2.918757     3.947616    -3.954479     127.89
 H      -3.323554     4.728554    -3.585179      27.04
 C      -2.612449     1.575079    -3.563533      58.04
 H      -2.292769     1.508955    -4.567662      25.10
 C      -3.367985     0.459612    -1.567395      41.18
 C      -3.697548    -0.906064    -0.800661      84.09
 H      -4.504473    -1.405569    -1.388522      24.98
 O      -4.460573    -0.600957     0.507833      85.77
 H      -3.876735    -0.093870     1.196787      22.62
 C      -2.495444    -1.726541    -0.534718     100.79
 H      -1.866286    -2.085608    -1.288831      26.18
 C      -2.748724    -3.144250     0.256112     100.35
 O      -3.598486    -4.001641    -0.510005     205.45
 H      -3.198118    -4.197729    -1.290295      33.73
 H      -3.432222    -2.901867     1.299171      23.31
 H      -1.822637    -3.616080     0.659621      26.51
 C       1.924266    -1.320508    -0.933303      30.07
 H       2.488651    -1.849156    -1.665264      21.43
 C       1.747643     0.524128     0.490080      47.81
 H       2.150982     1.578883     1.067518      20.46
 C       0.453579     0.263410     0.743626      17.06
 O      -0.259506     1.055271     1.679091     228.07
 C      -0.442861     2.474932     1.272266     109.64
 H      -0.984156     2.827219     2.259870      24.04
 H       0.624572     2.910255     1.736687      22.62
 H      -0.655206     2.434385     0.356227      29.21
 C      -0.282621    -0.855413     0.043383     -17.49
 O      -1.495925    -1.171576     0.407127     186.11
 C       0.621537    -1.722161    -0.648952      68.33
 H      -0.052264    -2.561015    -1.245530      23.53
 C       2.654891    -0.155832    -0.384085      18.35
 C       3.925379     0.308612    -0.924602      92.11
 H       3.867932    -0.219716    -2.053026      22.00
 O       3.973586     1.751977    -1.044376     213.83
 H       4.414413     2.203240    -0.234119      22.83
 C       5.187335    -0.218334    -0.155580      88.95
 H       5.166191     0.206266     0.928764      26.02
 O       5.075271    -1.629683    -0.023076     266.86
 H       5.275130    -2.032251    -0.929076      27.95
 C       6.676880     0.123245    -0.947454      94.94
 O       7.168861     1.437298    -0.895021     216.40
 H       7.351792     1.799138     0.050719      24.04
 H       6.471614    -0.208686    -1.927780      29.91
 H       7.278614    -0.643778    -0.318098      29.07
55
name= lig-ACN-Water-frame_496
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 C      -2.753973     0.404230    -2.929658      48.82
 H      -2.414620    -0.557443    -3.222820      26.35
 C      -3.768493     1.700615    -1.037371      50.40
 H      -3.909544     1.534878     0.080739      22.25
 C      -3.531583     2.886623    -1.696271      10.58
 O      -3.841231     4.209889    -1.130899     256.61
 C      -5.018362     4.263736    -0.410506     111.94
 H      -5.785842     3.905955    -1.168745      27.13
 H      -5.455915     5.281052    -0.286840      27.89
 H      -4.802480     3.999500     0.695019      27.99
 C      -3.087668     2.862502    -3.044597       6.72
 O      -2.871990     3.912452    -3.910301     145.50
 H      -3.445864     4.726429    -3.752526      20.02
 C      -2.595206     1.601692    -3.651912      46.66
 H      -2.361763     1.610613    -4.727286      24.89
 C      -3.394878     0.402634    -1.574686      18.91
 C      -3.707132    -0.798003    -0.696075      90.72
 H      -4.354561    -1.507499    -1.388692      25.36
 O      -4.443816    -0.620805     0.448541     197.96
 H      -3.829952    -0.121331     1.119686      24.77
 C      -2.417170    -1.844490    -0.476468      96.04
 H      -2.129572    -1.805598    -1.495305      28.34
 C      -2.818780    -3.096901     0.228016     107.05
 O      -3.675252    -4.119074    -0.424766     146.26
 H      -3.390114    -4.057934    -1.427781      29.56
 H      -3.394325    -2.757359     1.246501      24.10
 H      -1.801916    -3.587540     0.414501      25.67
 C       2.001213    -1.394666    -1.035068      53.29
 H       2.472792    -1.949183    -1.794031      25.21
 C       1.701168     0.625028     0.418686      17.54
 H       2.212060     1.679007     0.837646      20.58
 C       0.333679     0.219381     0.704310     -20.62
 O      -0.189539     1.066761     1.710763     152.20
 C      -0.452966     2.584297     1.355984      87.92
 H      -1.385202     3.024721     1.857218      23.88
 H       0.508108     3.208366     1.021782      23.91
 H      -0.967782     2.747347     0.510574      29.05
 C      -0.186059    -0.926481     0.126656     -22.85
 O      -1.634463    -1.045397     0.411999     129.17
 C       0.665494    -1.745185    -0.711274      49.88
 H       0.394530    -2.657324    -1.352515      27.35
 C       2.443486    -0.251124    -0.386749       5.06
 C       3.964667     0.256508    -0.860458     103.51
 H       4.154568    -0.159374    -1.997509      25.00
 O       3.927114     1.689683    -1.073045     241.22
 H       4.186305     2.051824    -0.243068      26.45
 C       5.298466    -0.208715    -0.249321      93.56
 H       5.480190     0.210556     0.861793      25.77
 O       5.048131    -1.658208    -0.057541     257.16
 H       5.175953    -2.063837    -0.950480      28.21
 C       6.571112     0.116705    -0.959183     104.83
 O       7.236628     1.436237    -0.849450     193.59
 H       7.460069     1.540014     0.089471      27.69
 H       6.688118     0.012239    -2.034018      27.96
 H       7.391961    -0.624045    -0.625037      28.95
55
name= lig-ACN-Water-frame_497
 C      -2.796402     0.404699    -2.896867      65.91
 H      -2.601706    -0.448194    -3.484297      21.82
 C      -3.721243     1.665680    -1.030521      57.55
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 H      -3.838550     1.882102     0.045136      19.67
 C      -3.538211     2.941011    -1.717406       4.47
 O      -3.760667     4.167297    -1.141568     250.09
 C      -5.082050     4.237318    -0.375981      92.04
 H      -5.911558     3.505459    -0.559060      26.51
 H      -5.140470     5.309885    -0.288463      26.37
 H      -4.934316     3.586098     0.595565      24.87
 C      -3.086623     2.819027    -3.062526      31.70
 O      -2.821839     3.890110    -3.872391     138.55
 H      -3.494827     4.628747    -3.555482      19.61
 C      -2.730819     1.622418    -3.622827      55.22
 H      -2.054473     1.754152    -4.535894      26.68
 C      -3.363297     0.453855    -1.642273      42.43
 C      -3.675680    -0.894642    -0.807220      84.45
 H      -4.536566    -1.522899    -1.378546      24.13
 O      -4.431157    -0.583797     0.464861     124.14
 H      -3.838356    -0.312100     1.220212      24.14
 C      -2.534810    -1.759746    -0.540116      80.55
 H      -1.845962    -2.152875    -1.296486      26.29
 C      -2.837073    -3.155630     0.251546      98.64
 O      -3.681750    -4.160546    -0.420130      91.71
 H      -3.484692    -4.145030    -1.493191      27.04
 H      -3.345216    -2.923450     1.264011      25.61
 H      -1.872624    -3.739954     0.588428      25.12
 C       1.972407    -1.434109    -1.058074      39.62
 H       2.677646    -2.021894    -1.607621      24.03
 C       1.671588     0.583349     0.291446      61.40
 H       2.098646     1.545335     0.859148      23.13
 C       0.416437     0.357632     0.745109     -25.44
 O      -0.265542     1.144587     1.704137     201.17
 C      -0.559838     2.527954     1.282639     113.86
 H      -0.812574     2.776523     2.378463      23.70
 H       0.406491     3.058409     1.310997      24.41
 H      -1.114263     2.416899     0.446812      29.05
 C      -0.178711    -0.976500     0.211311     -63.73
 O      -1.557717    -0.962689     0.406856      35.85
 C       0.568749    -1.802928    -0.802872      51.62
 H       0.062896    -2.685542    -1.038051      25.04
 C       2.570068    -0.217915    -0.495754      20.39
 C       3.903949     0.231215    -0.898341      92.28
 H       3.941958    -0.184176    -2.035015      23.28
 O       3.902331     1.690126    -1.085640     214.51
 H       3.999566     2.180831    -0.182214      23.35
 C       5.263135    -0.248982    -0.215480      80.14
 H       5.378244     0.176965     0.930772      24.03
 O       5.110473    -1.697837    -0.113479     284.84
 H       5.102081    -2.039789    -1.039143      28.39
 C       6.655931     0.082499    -1.064526      85.60
 O       7.266530     1.426076    -0.779456     236.19
 H       7.226337     1.794861     0.121957      26.05
 H       6.153121     0.023594    -2.059471      25.78
 H       7.293482    -0.783815    -0.791146      29.49
55
name= lig-ACN-Water-frame_498
 C      -2.908346     0.372883    -2.932204      47.36
 H      -2.597395    -0.573140    -3.341960      24.24
 C      -3.611299     1.726871    -0.977918      55.30
 H      -4.341979     1.588460    -0.232483      22.32
 C      -3.561905     2.864106    -1.765162      59.89
 O      -3.758580     4.109283    -1.170439     224.40
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 C      -5.057622     4.151181    -0.254137      98.41
 H      -5.748314     3.854500    -1.031514      21.09
 H      -5.377271     5.227055    -0.184264      25.71
 H      -4.815145     3.963946     0.840026      23.43
 C      -3.060260     2.851989    -3.079189       4.75
 O      -2.776070     3.932459    -3.848970      65.45
 H      -3.246124     4.878100    -3.609093      23.91
 C      -2.758984     1.569183    -3.604285      55.95
 H      -2.359043     1.483900    -4.701534      23.54
 C      -3.383166     0.403236    -1.564272      22.34
 C      -3.749701    -0.862644    -0.888476      73.26
 H      -4.531714    -1.509231    -1.629773      23.81
 O      -4.417086    -0.583164     0.427322     147.09
 H      -3.744749    -0.227466     1.030969      25.98
 C      -2.431840    -1.808736    -0.471781      72.86
 H      -2.037172    -1.941495    -1.538243      24.30
 C      -2.846651    -3.210646     0.316653     105.59
 O      -3.663826    -4.136434    -0.473075     187.82
 H      -3.227900    -4.230223    -1.320241      31.79
 H      -3.441903    -2.998874     1.180084      26.14
 H      -1.720446    -3.525600     0.524517      24.71
 C       1.881386    -1.442323    -1.009649      50.33
 H       2.333716    -2.214353    -1.641581      19.81
 C       1.797313     0.619655     0.277221      19.16
 H       2.333240     1.536927     0.599647      20.92
 C       0.458929     0.236273     0.707433      17.99
 O      -0.336904     1.066503     1.631723     221.36
 C      -0.615921     2.443784     1.309745     116.99
 H      -1.218608     3.087294     2.069800      24.88
 H       0.161865     2.972876     0.864714      27.56
 H      -1.416782     2.703006     0.639121      25.65
 C      -0.177777    -0.840385     0.149572      16.61
 O      -1.527332    -0.989491     0.372427     165.55
 C       0.501114    -1.732371    -0.671070      63.45
 H       0.132319    -2.523952    -1.134175      25.71
 C       2.511479    -0.274291    -0.582904      15.25
 C       3.954804     0.280583    -1.036854      90.71
 H       4.161785    -0.095478    -2.107037      24.21
 O       3.899472     1.740054    -1.088864     194.17
 H       4.283552     1.965808    -0.096284      22.91
 C       5.201137    -0.328353    -0.212059      77.96
 H       5.095753     0.038629     0.975936      24.14
 O       5.209701    -1.747618    -0.173051     256.04
 H       5.303305    -2.087817    -1.126068      26.83
 C       6.589393     0.135939    -1.053951      87.43
 O       7.251672     1.346467    -0.789942     216.65
 H       7.262253     1.460076     0.199109      28.18
 H       6.539397     0.267811    -2.211860      26.11
 H       7.344856    -0.657152    -1.061487      30.10
55
name= lig-ACN-Water-frame_499
 C      -3.000972     0.326093    -2.886020      58.32
 H      -2.840557    -0.669029    -3.342420      25.78
 C      -3.676231     1.622522    -0.967334      57.50
 H      -4.081570     1.731669    -0.005127      22.63
 C      -3.518547     2.855458    -1.730825      -1.66
 O      -3.852432     4.108299    -1.124347     255.12
 C      -4.944008     4.177818    -0.295650     122.49
 H      -5.827410     3.545694    -0.473088      25.61
 H      -5.096449     5.294376    -0.171073      25.69
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 H      -4.840674     3.525173     0.641196      23.99
 C      -3.007576     2.827282    -3.104567       3.30
 O      -2.701396     4.003708    -3.855639      23.78
 H      -3.520634     4.657751    -3.587116      21.63
 C      -2.748030     1.513096    -3.686004      43.42
 H      -2.632556     1.494478    -4.825786      23.69
 C      -3.377451     0.388602    -1.567610      36.72
 C      -3.724848    -0.855176    -0.746996      88.90
 H      -4.400863    -1.674524    -1.429424      23.29
 O      -4.453577    -0.620540     0.340841     191.89
 H      -3.931399    -0.145035     1.038784      24.85
 C      -2.424105    -1.874408    -0.463450      91.56
 H      -1.820891    -2.175502    -1.399048      25.06
 C      -2.781490    -3.134253     0.292323     121.34
 O      -3.589105    -4.068225    -0.532212     209.27
 H      -3.108978    -4.257375    -1.299917      32.03
 H      -3.282061    -2.875022     1.141281      28.26
 H      -2.028022    -3.905082     0.724455      25.19
 C       1.870726    -1.469937    -1.011418      49.04
 H       2.280968    -2.116024    -1.849992      21.75
 C       1.836979     0.594174     0.330461      60.92
 H       2.197356     1.466125     0.700635      25.51
 C       0.498193     0.319680     0.697682      -8.09
 O      -0.372184     0.920495     1.549561     187.54
 C      -0.726339     2.460641     1.224699      97.15
 H      -0.791036     2.742650     2.385191      23.45
 H       0.104340     2.906488     0.852280      28.01
 H      -1.521256     2.157452     0.567142      24.89
 C      -0.258391    -0.772183     0.037934      -3.63
 O      -1.613553    -1.038066     0.371457     168.57
 C       0.491900    -1.699834    -0.576618      63.69
 H       0.031038    -2.504875    -1.043444      25.13
 C       2.514193    -0.252126    -0.647079      19.31
 C       3.952493     0.213095    -1.161764      78.04
 H       4.096803     0.070617    -2.236810      24.80
 O       3.968030     1.765380    -1.028772     187.48
 H       4.516308     2.216873    -0.325005      25.62
 C       5.207427    -0.326732    -0.390346      82.66
 H       5.288313     0.090855     0.778794      24.64
 O       5.286355    -1.814650    -0.239834     217.13
 H       5.317080    -2.208424    -1.199757      26.78
 C       6.490132     0.105293    -1.043101      91.49
 O       7.229134     1.341849    -0.770782     200.26
 H       7.571303     1.534098     0.186362      26.05
 H       6.054572     0.087770    -2.145153      29.23
 H       7.078854    -0.752718    -0.804127      31.23
55
name= lig-ACN-Water-frame_500
 C      -3.013379     0.316888    -2.951101      55.59
 H      -3.091674    -0.623475    -3.572169      23.11
 C      -3.757360     1.664503    -0.997366      49.77
 H      -3.702815     1.766839     0.066067      21.11
 C      -3.455527     2.840634    -1.711716      14.78
 O      -3.832525     4.073596    -1.237574     186.64
 C      -4.944910     4.117432    -0.178708     106.32
 H      -5.830102     3.863534    -0.722010      27.89
 H      -5.053564     5.269620     0.036370      27.33
 H      -4.535351     3.886266     0.784179      28.54
 C      -2.946138     2.777308    -3.074517      11.16
 O      -2.682715     3.967938    -3.811991     171.06
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 H      -3.288232     4.802652    -3.609863      21.05
 C      -2.830786     1.517878    -3.676643      61.65
 H      -2.396743     1.400827    -4.663243      23.96
 C      -3.406882     0.337805    -1.560054      -1.27
 C      -3.585793    -1.044687    -0.805631      64.88
 H      -4.473441    -1.582050    -1.496336      22.49
 O      -4.572054    -0.645246     0.420766      58.29
 H      -4.007394    -0.129953     1.112952      26.29
 C      -2.425860    -1.841616    -0.484050      80.93
 H      -1.924702    -2.061338    -1.494310      24.55
 C      -2.775176    -3.149029     0.306683     113.07
 O      -3.549240    -3.983312    -0.576311     171.20
 H      -3.060303    -4.024763    -1.535035      26.20
 H      -3.434357    -2.955323     1.006391      27.50
 H      -1.699997    -3.350512     0.662521      24.68
 C       1.919751    -1.400805    -1.069965      34.54
 H       2.528212    -2.103086    -1.765670      20.16
 C       1.804169     0.550373     0.353821      56.36
 H       2.339783     1.193182     0.848621      25.37
 C       0.389569     0.295340     0.574030       2.64
 O      -0.368108     0.958479     1.546866     218.65
 C      -0.772276     2.306924     1.220804     103.51
 H      -1.069778     2.855628     2.183813      24.08
 H       0.009097     2.849630     0.683318      26.27
 H      -1.785805     2.638278     0.651000      21.25
 C      -0.295702    -0.799185     0.050304     -29.72
 O      -1.598468    -1.003330     0.427851     135.71
 C       0.521319    -1.797356    -0.692741      39.01
 H       0.081369    -2.837782    -0.816589      22.10
 C       2.557221    -0.193222    -0.622898       4.44
 C       3.872441     0.254593    -1.149408     119.17
 H       3.851765     0.022677    -2.134889      25.40
 O       4.046688     1.735554    -1.022601     228.28
 H       4.532610     1.729255    -0.232538      28.85
 C       5.158624    -0.366019    -0.468533      79.68
 H       4.950196     0.042822     0.693498      22.53
 O       5.298468    -1.814613    -0.308965     249.71
 H       5.251300    -2.226798    -1.262063      24.97
 C       6.535136     0.042724    -1.109996      99.31
 O       7.165995     1.347739    -0.805564     209.80
 H       7.049937     1.509666     0.190202      27.55
 H       6.695850     0.121116    -2.320377      23.93
 H       7.240822    -0.690733    -0.928199      30.80
55
name= lig-ACN-Water-frame_501
 C      -3.091742     0.314468    -2.967349      57.66
 H      -2.862707    -0.692902    -3.452368      23.61
 C      -3.644268     1.581643    -1.017820      61.71
 H      -4.290015     1.615126    -0.079640      20.81
 C      -3.485238     2.789457    -1.755681      35.70
 O      -3.804024     4.092228    -1.316215     168.20
 C      -4.860892     4.163517    -0.105652     106.92
 H      -5.711374     3.619602    -0.481796      24.89
 H      -4.980538     5.328960    -0.093459      23.65
 H      -4.782619     3.541688     0.704434      25.18
 C      -2.951898     2.791940    -3.039615      23.01
 O      -2.659420     3.885973    -3.754733     112.11
 H      -3.266573     4.548731    -3.407817      25.56
 C      -2.831510     1.523169    -3.643388      59.71
 H      -2.544033     1.572231    -4.636938      24.67
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 C      -3.457322     0.325919    -1.615944      36.82
 C      -3.797057    -0.925912    -0.839509      76.83
 H      -4.199497    -1.906315    -1.507497      22.32
 O      -4.575965    -0.742117     0.435903     143.61
 H      -3.991798    -0.146836     0.995425      23.66
 C      -2.417125    -1.769448    -0.409089      70.38
 H      -1.798566    -1.947757    -1.334495      25.33
 C      -2.768229    -3.100927     0.277880     117.31
 O      -3.498015    -3.961208    -0.634743     193.06
 H      -3.064751    -3.880408    -1.645447      24.17
 H      -3.221009    -2.935189     1.141758      28.57
 H      -1.953446    -3.835917     0.568555      25.68
 C       1.885523    -1.350796    -1.112276      52.40
 H       2.548971    -2.108838    -1.652065      19.25
 C       1.716379     0.542463     0.374844      58.10
 H       2.001528     1.327841     0.933818      22.90
 C       0.345747     0.263198     0.505983     -59.44
 O      -0.358226     1.012658     1.585069     149.17
 C      -0.838824     2.360541     1.218004      85.78
 H      -0.810563     2.909777     2.202861      23.04
 H      -0.017034     2.713393     0.481881      23.75
 H      -1.787916     1.917792     0.531821      21.82
 C      -0.177554    -0.992543    -0.017519     -17.07
 O      -1.547306    -0.992279     0.440226     125.38
 C       0.616257    -1.783266    -0.788128      75.33
 H       0.418794    -2.934095    -1.170137      23.69
 C       2.423523    -0.225963    -0.540131      24.31
 C       3.856971     0.268670    -1.148001     104.79
 H       3.905811     0.149188    -2.116535      28.39
 O       4.120317     1.661791    -1.020325     214.64
 H       4.225525     2.080477    -0.077464      24.68
 C       5.156904    -0.421952    -0.506074      75.07
 H       5.373536    -0.001867     0.632576      24.92
 O       5.204443    -1.796188    -0.355035     274.87
 H       5.429367    -2.231379    -1.257470      26.39
 C       6.707012     0.047694    -1.210621      87.17
 O       7.041698     1.363458    -0.845449     211.41
 H       7.192201     1.484319     0.123660      26.56
 H       6.480840    -0.112189    -2.428686      27.44
 H       7.312992    -0.657238    -0.798165      33.56
55
name= lig-ACN-Water-frame_502
 C      -3.103794     0.263663    -2.984062      57.75
 H      -2.890669    -0.693256    -3.561631      23.36
 C      -3.661146     1.568188    -1.006770      52.07
 H      -4.408534     1.569161    -0.085293      19.91
 C      -3.540596     2.794784    -1.703972      24.98
 O      -3.834593     4.088291    -1.236651     242.82
 C      -4.739260     4.148972    -0.220462     128.12
 H      -5.746442     3.823762    -0.443881      26.06
 H      -4.882879     5.256537     0.193339      25.73
 H      -4.201839     3.886288     0.562459      28.15
 C      -2.982553     2.699811    -3.014342       9.57
 O      -2.646631     3.892595    -3.721621     137.27
 H      -3.252976     4.617394    -3.586992      25.54
 C      -2.777370     1.471931    -3.686193      51.88
 H      -2.602396     1.438466    -4.713859      23.99
 C      -3.556866     0.319186    -1.660265      21.63
 C      -3.832510    -0.922643    -0.763669      86.47
 H      -4.738322    -1.508064    -1.449616      21.09
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 O      -4.559463    -0.825105     0.379325     171.37
 H      -4.148493    -0.395136     1.139666      23.56
 C      -2.457202    -1.709255    -0.410593      83.61
 H      -2.052641    -1.965437    -1.410420      25.35
 C      -2.727819    -3.127081     0.241239     110.33
 O      -3.537685    -3.945235    -0.687450     207.31
 H      -3.033872    -4.017811    -1.576224      27.51
 H      -3.391929    -3.068168     1.029623      26.09
 H      -1.693502    -3.435329     0.511579      25.77
 C       1.945957    -1.389369    -1.150869      44.99
 H       2.567179    -1.820237    -1.985862      19.43
 C       1.619789     0.610512     0.363999      53.16
 H       2.041511     1.547385     0.699589      21.35
 C       0.347306     0.227380     0.652280      37.61
 O      -0.293681     0.933409     1.577021     177.16
 C      -0.855643     2.370844     1.112714      73.11
 H      -1.048604     2.901207     2.076235      24.72
 H      -0.195611     3.100028     0.367553      23.44
 H      -2.113251     2.470067     0.747889      22.81
 C      -0.184329    -0.939978     0.052173     -14.31
 O      -1.471320    -1.061633     0.405563     175.59
 C       0.611908    -1.847200    -0.860710      54.49
 H      -0.052121    -2.692691    -1.586229      20.75
 C       2.516077    -0.153194    -0.548295      12.10
 C       3.925754     0.205644    -1.044052     102.09
 H       3.783314    -0.092363    -1.983347      26.51
 O       4.127217     1.699821    -1.008184     191.13
 H       4.116242     1.837083     0.038455      25.04
 C       5.332279    -0.375042    -0.550375      79.21
 H       5.335519     0.105979     0.563709      25.61
 O       5.081528    -1.859091    -0.358438     308.56
 H       5.156817    -2.288317    -1.271660      28.05
 C       6.610594    -0.010568    -1.190945     105.55
 O       6.982299     1.433231    -0.928907     120.76
 H       7.270349     1.485611     0.015383      29.11
 H       6.735774    -0.034663    -2.465562      28.13
 H       7.352502    -0.641273    -0.926222      34.73
55
name= lig-ACN-Water-frame_503
 C      -3.073433     0.217753    -2.998106      57.95
 H      -3.226605    -0.784402    -3.475143      22.51
 C      -3.881714     1.607950    -0.990705      43.80
 H      -3.855577     1.593636     0.208304      25.24
 C      -3.530150     2.773845    -1.717915      11.67
 O      -3.786165     4.056757    -1.294781     176.24
 C      -4.670175     4.210944    -0.098579     113.13
 H      -5.580747     3.608816    -0.314134      25.34
 H      -4.780393     5.350278    -0.145087      25.78
 H      -4.434230     3.721633     0.724339      26.64
 C      -3.003506     2.734468    -3.053516      -1.60
 O      -2.650530     3.881912    -3.701143      70.74
 H      -3.317440     4.631490    -3.466955      22.01
 C      -2.790167     1.403221    -3.674674      48.76
 H      -2.276227     1.405095    -4.648563      24.69
 C      -3.588939     0.332835    -1.608273     -26.74
 C      -3.741861    -0.984125    -0.790013      66.11
 H      -4.179624    -1.928607    -1.570981      21.82
 O      -4.656946    -0.822754     0.461939     116.25
 H      -3.987466    -0.585559     1.153898      25.56
 C      -2.531508    -1.820913    -0.581033      86.25
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 H      -2.000028    -1.875899    -1.524840      26.66
 C      -2.760137    -3.123891     0.153649     123.18
 O      -3.570568    -3.954042    -0.672017     259.42
 H      -3.204034    -4.071114    -1.511954      30.80
 H      -3.173910    -2.992570     1.165665      26.49
 H      -1.821795    -3.636603     0.395915      27.34
 C       1.944640    -1.341456    -1.134566      53.79
 H       2.351952    -1.816557    -2.016200      24.79
 C       1.807680     0.648519     0.218222      12.00
 H       2.104619     1.666364     0.692597      22.15
 C       0.505922     0.145560     0.723272     -20.48
 O      -0.398977     1.025844     1.582834     111.63
 C      -0.896750     2.348776     1.142064      94.48
 H      -0.755117     2.984465     2.046296      26.47
 H       0.002357     2.678997     0.263953      25.55
 H      -1.977339     2.080340     0.428084      25.39
 C      -0.141083    -0.959265     0.038679      -7.49
 O      -1.539653    -1.127030     0.388806     110.97
 C       0.595437    -1.667536    -0.856556      66.20
 H      -0.028209    -2.511297    -1.618270      23.01
 C       2.554705    -0.223970    -0.528029      33.01
 C       4.013211     0.266869    -1.039247     103.50
 H       4.194577     0.076796    -2.044808      30.82
 O       4.070121     1.711699    -0.951723     187.62
 H       4.607062     2.011776    -0.201754      26.59
 C       5.245305    -0.454690    -0.418448      85.89
 H       5.575664    -0.244435     0.692006      27.56
 O       5.021189    -1.863996    -0.347042     297.80
 H       5.083312    -2.298708    -1.232425      29.50
 C       6.605658     0.040899    -1.222828      83.07
 O       6.969361     1.438582    -1.019998     202.69
 H       6.869971     1.703121    -0.042833      26.12
 H       6.365793    -0.124409    -2.484663      25.35
 H       7.316139    -0.552089    -0.867400      32.55
55
name= lig-ACN-Water-frame_504
 C      -3.172449     0.247270    -2.847094      68.55
 H      -2.901635    -0.679642    -3.378768      26.52
 C      -3.936047     1.571108    -1.044137      50.05
 H      -4.217292     1.748167     0.108556      26.20
 C      -3.580953     2.717734    -1.779221       6.49
 O      -3.719401     4.049625    -1.287341     163.10
 C      -4.638072     4.240590    -0.036955     108.00
 H      -5.630297     3.752836    -0.274623      25.09
 H      -4.889150     5.329899     0.145191      27.10
 H      -4.130553     4.060110     0.757400      29.31
 C      -3.020627     2.654287    -3.078902      14.32
 O      -2.665844     3.874439    -3.711847      85.30
 H      -3.272363     4.667287    -3.304348      22.06
 C      -2.787590     1.427600    -3.615451      53.32
 H      -2.323955     1.321026    -4.668173      21.36
 C      -3.601124     0.295723    -1.568390      12.89
 C      -3.807678    -1.009945    -0.803623      64.13
 H      -4.727633    -1.671161    -1.420295      20.11
 O      -4.641365    -0.843376     0.419925     108.71
 H      -4.172097    -0.426514     1.248098      24.59
 C      -2.381652    -1.845406    -0.612304      86.85
 H      -1.971449    -2.094614    -1.569131      27.21
 C      -2.733471    -3.201753     0.056296     112.89
 O      -3.708734    -4.034380    -0.634914     230.48
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 H      -3.322857    -4.111359    -1.479927      32.62
 H      -3.253065    -2.887469     1.048437      25.07
 H      -1.811596    -3.681424     0.162097      27.67
 C       1.922471    -1.304013    -1.179904      38.87
 H       2.471324    -2.006537    -1.726098      24.57
 C       1.843205     0.588523     0.288618      33.85
 H       2.446936     1.595282     0.590676      21.27
 C       0.547978     0.259989     0.690164     -10.58
 O      -0.427662     0.996046     1.603092     168.46
 C      -0.771871     2.248353     1.078191      98.54
 H      -1.031176     3.075509     1.849925      25.55
 H      -0.083341     2.804009     0.119209      25.15
 H      -2.074170     2.276134     0.691294      26.12
 C      -0.196058    -0.869710     0.149768      -2.46
 O      -1.555977    -1.152324     0.338008     131.10
 C       0.579257    -1.524019    -0.902145      53.19
 H       0.243141    -2.603951    -1.482988      22.69
 C       2.699539    -0.222742    -0.620048       8.10
 C       4.021550     0.290389    -1.022698      94.77
 H       4.023122     0.022117    -2.062459      27.21
 O       4.034533     1.770003    -0.898492     164.60
 H       4.589830     2.027718    -0.160967      28.46
 C       5.208535    -0.458221    -0.276065      89.86
 H       5.156706    -0.103839     0.815311      28.05
 O       5.008802    -1.894527    -0.358776     301.20
 H       5.207999    -2.175380    -1.292669      29.87
 C       6.557716     0.022557    -1.181177      85.06
 O       6.928221     1.443108    -1.096594     152.35
 H       7.011969     1.577353    -0.072842      27.46
 H       6.264084    -0.166782    -2.412373      26.64
 H       7.378794    -0.552742    -1.064880      32.09
55
name= lig-ACN-Water-frame_505
 C      -3.115038     0.257586    -2.861256      57.96
 H      -2.777065    -0.721360    -3.160890      24.39
 C      -3.934404     1.575812    -1.030001      44.16
 H      -4.819908     1.597480    -0.295287      19.54
 C      -3.683382     2.764401    -1.769734      30.56
 O      -3.746335     4.040200    -1.183969     244.93
 C      -4.524836     4.277892    -0.092165     132.57
 H      -5.477522     3.650823     0.106967      24.15
 H      -4.643532     5.330847    -0.144769      26.50
 H      -4.086738     3.884329     0.690997      29.12
 C      -3.052667     2.710642    -3.048522       9.07
 O      -2.681642     3.815790    -3.730743      -8.21
 H      -3.281226     4.680892    -3.457352      22.58
 C      -2.816348     1.368994    -3.580362      48.40
 H      -2.459015     1.189145    -4.663183      22.90
 C      -3.669922     0.266449    -1.488940      -8.70
 C      -3.901381    -1.017419    -0.790352      74.51
 H      -4.506285    -1.780060    -1.653893      21.83
 O      -4.593995    -0.881254     0.374077     196.87
 H      -3.912969    -0.328610     0.950287      23.68
 C      -2.397560    -1.878612    -0.627450      73.28
 H      -1.897065    -1.733593    -1.548654      24.58
 C      -2.693016    -3.293780     0.014445      99.10
 O      -3.843962    -4.096035    -0.621404     156.27
 H      -3.633460    -4.395446    -1.614055      26.91
 H      -3.173374    -3.181383     1.119010      24.21
 H      -1.868345    -3.879807     0.236523      27.26
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 C       1.985794    -1.287107    -1.214301      41.30
 H       2.444138    -1.934088    -1.891393      20.41
 C       1.866899     0.516627     0.418359      35.41
 H       2.273371     1.494768     1.010179      18.65
 C       0.393402     0.311726     0.657502     -30.17
 O      -0.288249     0.925286     1.613894     179.76
 C      -0.798683     2.331980     1.017775      49.05
 H      -0.532706     2.940936     1.969539      21.26
 H       0.142193     2.602106     0.122099      22.41
 H      -1.941691     2.010500     0.361435      20.51
 C      -0.142855    -0.783479     0.012221      15.63
 O      -1.497395    -1.102386     0.328041     166.44
 C       0.575948    -1.522867    -0.874950      55.55
 H      -0.106808    -2.439762    -1.263416      19.79
 C       2.531928    -0.141813    -0.596376      31.80
 C       3.997208     0.283966    -1.015805      79.43
 H       4.227603     0.093371    -2.093819      24.67
 O       4.040976     1.817968    -0.868945     171.85
 H       4.170765     1.942140     0.159596      23.40
 C       5.227090    -0.361921    -0.334388      93.77
 H       5.302586    -0.199778     0.733035      28.54
 O       5.045746    -1.890182    -0.369912     288.45
 H       5.124358    -2.252057    -1.317510      29.03
 C       6.480105    -0.043514    -1.075147      97.32
 O       6.864777     1.418259    -1.090165     127.85
 H       7.362686     1.620208    -0.277069      32.45
 H       6.108800    -0.188253    -2.265563      29.08
 H       7.281950    -0.663462    -0.837839      32.86
55
name= lig-ACN-Water-frame_506
 C      -3.001076     0.164317    -2.789597      73.01
 H      -2.976432    -0.716144    -3.373237      24.72
 C      -4.089686     1.585560    -0.993639      69.78
 H      -4.531589     1.654755     0.014638      20.30
 C      -3.705814     2.749791    -1.708191      16.33
 O      -3.755390     4.019334    -1.237455     212.43
 C      -4.473786     4.300486     0.048060     122.37
 H      -5.469173     3.843402    -0.236430      25.04
 H      -4.651521     5.337450     0.089902      27.92
 H      -3.981211     4.141284     0.866751      29.50
 C      -3.110836     2.658158    -3.008897      11.48
 O      -2.698305     3.780609    -3.780387     129.45
 H      -3.255800     4.625941    -3.484322      21.25
 C      -2.867155     1.412662    -3.570499      44.33
 H      -2.319480     1.502229    -4.541210      21.82
 C      -3.652741     0.320541    -1.615481      17.67
 C      -3.797017    -1.094800    -0.862061      73.18
 H      -4.477875    -2.026489    -1.476334      21.64
 O      -4.599775    -0.926522     0.409531     165.69
 H      -4.041841    -0.710490     1.242080      21.36
 C      -2.507904    -1.830468    -0.599190      78.04
 H      -2.090589    -2.136824    -1.543406      22.25
 C      -2.748788    -3.407703    -0.028156     102.81
 O      -3.902926    -4.096552    -0.585849     159.69
 H      -3.452948    -4.227387    -1.602386      25.52
 H      -2.871308    -3.122772     1.171249      22.97
 H      -1.923540    -3.937085    -0.285001      26.50
 C       1.903887    -1.247376    -1.210169      52.29
 H       2.422516    -1.566883    -2.086539      20.93
 C       1.744744     0.539175     0.539528      52.69
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 H       2.264102     1.208197     1.312844      19.55
 C       0.470945     0.238649     0.641650      -0.61
 O      -0.234037     1.049919     1.633294     170.17
 C      -0.685153     2.271246     1.043237      77.41
 H      -0.967571     3.185424     1.802450      22.15
 H       0.087572     2.664563     0.049535      21.75
 H      -1.999607     2.278925     0.618213      20.00
 C      -0.230189    -0.781041    -0.193587     -19.34
 O      -1.490239    -1.068454     0.306601     137.74
 C       0.642959    -1.674319    -0.930878      65.52
 H       0.308048    -2.536395    -1.565611      21.57
 C       2.501043    -0.128333    -0.542741       7.54
 C       3.897192     0.400524    -0.969677      90.64
 H       3.879693     0.220641    -2.121088      22.59
 O       4.032721     1.786187    -0.855045     218.64
 H       4.342602     2.166113     0.123320      21.06
 C       5.152705    -0.419867    -0.353916      95.41
 H       5.288976    -0.109825     0.646063      28.04
 O       5.103213    -1.815048    -0.379108     288.60
 H       5.016883    -2.102304    -1.339658      28.31
 C       6.484333    -0.019317    -1.083756     103.89
 O       6.845901     1.341003    -1.047829     207.32
 H       6.913883     1.590628    -0.090389      29.28
 H       6.571529    -0.449656    -2.237814      28.36
 H       7.175876    -0.589563    -0.501875      30.89
55
name= lig-ACN-Water-frame_507
 C      -2.987952     0.248064    -2.896652      60.40
 H      -2.656730    -0.699521    -3.251498      24.07
 C      -4.134402     1.478144    -1.020413      68.73
 H      -4.165716     1.481082     0.009299      24.16
 C      -3.703949     2.701298    -1.682323      -2.81
 O      -3.772593     4.086525    -1.216439     173.35
 C      -4.484345     4.339609     0.095473     125.09
 H      -5.498206     3.884163     0.370827      27.04
 H      -4.481952     5.372148     0.143859      28.54
 H      -3.982116     3.800021     0.748023      28.59
 C      -3.166137     2.636615    -3.006283      14.85
 O      -2.759795     3.711189    -3.773432     156.49
 H      -3.100953     4.600138    -3.460300      23.15
 C      -2.809549     1.407382    -3.574812      66.56
 H      -2.387678     1.342421    -4.552596      24.16
 C      -3.677323     0.242033    -1.556505     -21.05
 C      -3.800791    -1.041685    -0.759263      81.19
 H      -4.576059    -1.621700    -1.615137      21.25
 O      -4.625054    -1.015597     0.403874     209.98
 H      -4.043056    -0.633415     1.086282      26.72
 C      -2.510703    -1.928307    -0.586800      90.09
 H      -1.997207    -1.891805    -1.562355      22.99
 C      -2.750017    -3.342299    -0.023487     120.79
 O      -3.906071    -4.046315    -0.573114     210.04
 H      -3.849187    -4.259390    -1.545047      31.19
 H      -2.813659    -3.847213     1.105849      23.36
 H      -1.883879    -3.827737    -0.341026      26.85
 C       1.936723    -1.113193    -1.229378      53.52
 H       2.566859    -1.632526    -1.987876      21.29
 C       1.814829     0.499188     0.543361      35.65
 H       2.255947     1.266757     1.145182      20.42
 C       0.364515     0.192293     0.682525      -9.67
 O      -0.208965     1.096725     1.617460     153.40
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 C      -0.695673     2.330307     1.054814      74.37
 H      -0.554468     3.031064     2.048395      22.34
 H       0.100990     2.828882     0.134148      22.77
 H      -1.790345     1.902605     0.394340      20.85
 C      -0.267411    -0.892363    -0.184904     -19.93
 O      -1.606472    -1.106467     0.184421     171.36
 C       0.570520    -1.740528    -1.027126      47.59
 H       0.212500    -2.573006    -1.537683      21.42
 C       2.550225    -0.122626    -0.434046      36.62
 C       3.801931     0.365328    -0.966473      94.42
 H       3.790276     0.157898    -2.134388      23.27
 O       3.993521     1.839961    -0.861327     197.64
 H       4.331325     1.948800     0.176341      21.99
 C       5.081363    -0.342645    -0.416371     101.39
 H       5.053117    -0.125771     0.588150      28.38
 O       5.098506    -1.810778    -0.404560     272.31
 H       5.105492    -2.199437    -1.307102      29.06
 C       6.536957    -0.074983    -1.027529     100.49
 O       6.877143     1.334195    -0.998510     215.21
 H       6.764947     1.634791    -0.039631      29.11
 H       6.666662    -0.411283    -2.178865      27.91
 H       7.284994    -0.658083    -0.511511      31.23
55
name= lig-ACN-Water-frame_508
 C      -3.074864     0.203683    -2.828745      63.31
 H      -2.490878    -0.613003    -3.204465      25.41
 C      -3.984061     1.459291    -1.009478      68.66
 H      -4.672479     1.474302    -0.256437      26.70
 C      -3.750178     2.735086    -1.689283      10.79
 O      -3.890044     4.049652    -1.154261     179.28
 C      -4.418707     4.283803     0.135515     131.26
 H      -5.489841     4.022661    -0.060775      25.18
 H      -4.305647     5.329262     0.277448      28.02
 H      -3.930411     3.924854     0.945004      27.88
 C      -3.180726     2.643641    -3.019623       7.19
 O      -2.834191     3.698896    -3.766199     106.09
 H      -3.293184     4.501935    -3.473308      25.52
 C      -2.759850     1.385363    -3.598578      37.15
 H      -2.340495     1.428681    -4.561317      20.16
 C      -3.607342     0.226612    -1.566748      27.00
 C      -3.928610    -1.094586    -0.791411      85.11
 H      -4.518092    -1.969773    -1.480362      24.14
 O      -4.645357    -1.061114     0.438200     212.23
 H      -4.246848    -0.571353     1.164662      27.20
 C      -2.548517    -1.943223    -0.662369      93.62
 H      -2.272753    -2.238032    -1.715192      27.18
 C      -2.666256    -3.408288    -0.052937     105.60
 O      -3.936837    -3.980838    -0.586106     211.85
 H      -3.639106    -4.075564    -1.430141      35.43
 H      -2.788227    -2.921165     1.070900      24.56
 H      -1.837529    -4.100742    -0.242710      27.41
 C       1.871004    -1.211463    -1.238416      38.42
 H       2.503505    -1.741887    -2.043554      21.42
 C       1.726452     0.451880     0.561020      71.20
 H       1.936984     1.346600     1.001434      25.39
 C       0.387924     0.142858     0.651954     -23.51
 O      -0.224788     1.002666     1.589688     137.55
 C      -0.695577     2.373630     1.044430      72.02
 H      -1.044048     3.100002     1.975059      23.72
 H       0.241054     2.777989     0.274463      24.45
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 H      -1.868098     2.621928     0.477463      25.75
 C      -0.217813    -0.965275     0.022314      12.05
 O      -1.660024    -1.122055     0.130557     129.30
 C       0.553183    -1.519500    -1.027785      75.21
 H       0.225843    -2.267316    -1.542705      27.79
 C       2.478023    -0.214170    -0.458339      -0.96
 C       3.921412     0.375369    -1.062678      67.17
 H       3.872920     0.247985    -2.288309      24.75
 O       3.911965     1.836697    -0.896765     222.15
 H       4.162088     2.187210     0.066233      22.19
 C       5.164344    -0.353506    -0.425285     105.82
 H       5.169444    -0.080971     0.550451      30.52
 O       5.010976    -1.847872    -0.436911     273.04
 H       5.184489    -2.158621    -1.359612      29.84
 C       6.517305    -0.036791    -0.956451     109.29
 O       6.942733     1.343989    -0.962373     223.39
 H       7.322044     1.615191    -0.060314      26.78
 H       6.409136    -0.351125    -2.073333      30.41
 H       7.148904    -0.772164    -0.440374      31.40
55
name= lig-ACN-Water-frame_509
 C      -2.976258     0.126927    -2.841689      53.83
 H      -3.013313    -0.851245    -3.349126      23.83
 C      -3.940035     1.542281    -0.953698      44.27
 H      -4.588822     1.571487    -0.141039      18.67
 C      -3.745433     2.697926    -1.725008      24.61
 O      -3.936131     3.947429    -1.206214     170.33
 C      -4.453113     4.221765     0.195084     115.50
 H      -5.536426     4.028499     0.395936      26.05
 H      -4.390191     5.346862     0.248375      25.92
 H      -3.999212     3.596856     0.864076      26.56
 C      -3.162543     2.606984    -2.992612      16.72
 O      -2.904127     3.767070    -3.815670     167.74
 H      -3.320208     4.653318    -3.582179      19.83
 C      -2.838595     1.368515    -3.499008      62.39
 H      -2.226915     1.326524    -4.379531      27.96
 C      -3.629458     0.215351    -1.533439     -25.82
 C      -3.927504    -1.271921    -0.868635      63.74
 H      -4.851004    -1.703509    -1.494913      22.32
 O      -4.703417    -1.061571     0.483884     122.22
 H      -3.929355    -0.732376     1.057521      26.58
 C      -2.556059    -2.001450    -0.828979      67.36
 H      -2.030998    -1.858641    -1.819737      23.79
 C      -2.713186    -3.318986    -0.033576     112.07
 O      -3.881305    -3.921878    -0.591613     149.42
 H      -3.785636    -4.342548    -1.500402      28.16
 H      -2.961145    -3.333114     1.162669      25.22
 H      -1.757495    -3.951185    -0.047962      27.14
 C       1.868746    -1.309846    -1.216045      34.88
 H       2.198611    -1.797615    -2.222540      22.23
 C       1.738709     0.418654     0.421286      59.44
 H       2.257882     1.192793     0.937250      25.48
 C       0.356805     0.125479     0.756771     -13.07
 O      -0.423494     0.982652     1.553559     180.69
 C      -0.689075     2.357652     1.097016      92.64
 H      -0.685719     2.914181     2.146773      24.49
 H       0.232757     2.931974     0.497211      25.63
 H      -1.552545     2.013343     0.206102      26.11
 C      -0.300784    -0.968236     0.093151      10.43
 O      -1.615325    -1.095183     0.144566      93.27
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 C       0.462878    -1.477628    -1.012741      61.52
 H      -0.103646    -1.956443    -1.654463      27.13
 C       2.581342    -0.216970    -0.598276       4.71
 C       3.903834     0.376629    -1.036243      78.73
 H       4.025078     0.030591    -2.239959      26.34
 O       3.849126     1.812632    -0.945757     206.27
 H       4.410210     2.006686    -0.226245      27.52
 C       5.125270    -0.414416    -0.328252      95.14
 H       5.125107    -0.243816     0.690332      29.47
 O       4.924470    -1.815607    -0.474548     307.70
 H       5.006442    -2.189762    -1.416140      28.85
 C       6.560492    -0.007740    -1.009045     104.99
 O       7.049343     1.343475    -0.908598     246.99
 H       7.183443     1.529593     0.088077      25.43
 H       6.723903    -0.296567    -2.067631      29.77
 H       7.351210    -0.548023    -0.480311      30.43
55
name= lig-ACN-Water-frame_510
 C      -3.046704     0.143321    -2.746645      64.74
 H      -2.944467    -0.751890    -3.416818      25.17
 C      -3.974768     1.391772    -0.941526      75.13
 H      -3.973462     1.485003     0.130244      24.48
 C      -3.711945     2.644013    -1.662139      -8.34
 O      -4.023230     3.952130    -1.219779     179.84
 C      -4.513857     4.098823     0.182694     114.44
 H      -5.552236     3.764784     0.260087      25.28
 H      -4.181690     5.187137     0.410262      25.26
 H      -3.798642     3.635187     0.826012      26.75
 C      -3.133632     2.678676    -3.046203      -1.11
 O      -2.954891     3.722401    -3.855248     126.23
 H      -3.208671     4.579283    -3.383196      22.49
 C      -2.794984     1.321213    -3.504326      31.68
 H      -2.513811     1.304521    -4.592649      21.02
 C      -3.664426     0.150461    -1.492974      37.60
 C      -3.975887    -1.112365    -0.855477      96.73
 H      -4.473902    -1.847656    -1.592961      24.99
 O      -4.620042    -1.103276     0.406139     197.78
 H      -4.062225    -0.809750     1.235525      22.26
 C      -2.521451    -1.945374    -0.731695      78.58
 H      -2.069890    -2.258113    -1.740511      24.36
 C      -2.738484    -3.252038    -0.063018     107.34
 O      -3.874428    -3.982484    -0.606979     148.01
 H      -3.399206    -4.300461    -1.565014      25.80
 H      -2.985126    -2.889852     1.008925      25.45
 H      -1.765087    -3.949839    -0.147891      24.44
 C       1.809267    -1.303517    -1.295659      45.80
 H       2.334911    -1.868120    -2.149176      20.56
 C       1.763460     0.434402     0.336730      28.50
 H       2.243570     1.290192     0.904309      20.42
 C       0.403068     0.127378     0.798909      -2.15
 O      -0.560501     0.912138     1.574357     190.27
 C      -0.646069     2.252927     1.132805     107.98
 H      -1.225856     2.952133     1.900290      24.58
 H       0.350977     2.596625     0.604299      24.59
 H      -1.511000     2.682630     0.438712      25.35
 C      -0.274960    -0.864750    -0.024678     -16.40
 O      -1.731354    -1.089680     0.179642     124.19
 C       0.419505    -1.590668    -0.982082      62.86
 H       0.015475    -2.158562    -1.786658      22.28
 C       2.442101    -0.290402    -0.653565      35.55
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 C       3.888634     0.260135    -1.006831      77.61
 H       4.108433     0.089312    -2.232587      22.48
 O       3.878574     1.784279    -0.993197     208.58
 H       4.217514     2.109965    -0.159627      25.55
 C       5.105668    -0.388561    -0.341077      96.16
 H       5.170104    -0.208713     0.697291      27.73
 O       4.861414    -1.807929    -0.484364     300.16
 H       4.839345    -2.043104    -1.485762      27.51
 C       6.672829    -0.037695    -0.986013      91.45
 O       7.106170     1.375542    -0.863022     253.64
 H       7.082131     1.715168     0.079943      25.18
 H       6.463757    -0.229180    -1.974504      32.11
 H       7.301278    -0.881751    -0.598936      30.63
55
name= lig-ACN-Water-frame_511
 C      -3.155732     0.202096    -2.822934      66.88
 H      -2.683675    -0.783364    -3.054496      23.54
 C      -3.905723     1.444648    -0.905627      63.11
 H      -4.329954     1.389808     0.170186      22.32
 C      -3.687892     2.611500    -1.655060      16.64
 O      -4.101831     3.936419    -1.204074     212.72
 C      -4.475495     3.971008     0.138235     118.30
 H      -5.458642     3.499771     0.268345      26.30
 H      -4.836667     5.092215     0.418379      25.41
 H      -3.914767     3.462511     0.843677      28.75
 C      -3.153393     2.525061    -2.962666      13.90
 O      -2.984346     3.674421    -3.877240     121.63
 H      -3.314604     4.608441    -3.503896      22.65
 C      -2.791382     1.354876    -3.535355      61.54
 H      -2.438320     1.160236    -4.605122      19.96
 C      -3.681658     0.200269    -1.556839      -3.07
 C      -3.837880    -1.159917    -0.814404     105.54
 H      -4.570352    -1.720424    -1.454169      24.24
 O      -4.577201    -1.144935     0.372311     221.94
 H      -4.030424    -0.674197     1.053518      27.31
 C      -2.567182    -1.813522    -0.643065      83.17
 H      -2.085036    -1.740606    -1.685828      22.89
 C      -2.774957    -3.248963     0.021348      98.83
 O      -3.830867    -4.075809    -0.646545     195.16
 H      -3.606010    -4.275122    -1.685657      25.96
 H      -3.025944    -3.231197     1.123241      24.78
 H      -1.710924    -3.876517     0.009573      23.81
 C       1.690475    -1.335785    -1.404840      44.95
 H       2.295988    -1.974381    -2.083496      20.18
 C       1.653957     0.489795     0.438446      49.33
 H       2.193372     1.493114     0.821991      19.88
 C       0.316267     0.118314     0.646533      22.70
 O      -0.560882     0.775862     1.584166     175.65
 C      -0.695902     2.290528     1.161201     102.67
 H      -0.785805     2.739893     2.186304      24.83
 H       0.346436     2.570231     0.964513      27.21
 H      -1.138187     2.142430     0.115702      26.66
 C      -0.359784    -0.847805    -0.131446       2.49
 O      -1.676156    -1.044465     0.194197     172.03
 C       0.438557    -1.711019    -1.057812      51.91
 H      -0.107750    -2.697730    -1.280395      20.06
 C       2.371043    -0.254684    -0.601303      -9.08
 C       3.880123     0.275642    -1.077745      67.50
 H       3.834881    -0.090241    -2.290404      21.72
 O       3.936355     1.717475    -1.007229     225.92
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 H       4.073871     1.912074     0.021547      24.27
 C       5.190229    -0.373745    -0.369181      97.67
 H       5.099062    -0.090467     0.676220      28.82
 O       4.853097    -1.807994    -0.445762     289.44
 H       4.883728    -2.137140    -1.420901      26.88
 C       6.553152    -0.019989    -0.958097     117.37
 O       7.123781     1.329241    -0.823457     201.16
 H       7.403556     1.445324     0.119186      28.19
 H       6.651218    -0.103799    -1.936193      33.97
 H       7.392619    -0.674428    -0.526094      30.86
55
name= lig-ACN-Water-frame_512
 C      -3.132581     0.123474    -2.929256      55.60
 H      -2.975386    -0.825086    -3.511031      22.82
 C      -3.873177     1.504436    -0.877028      59.01
 H      -4.734216     1.584170    -0.073296      17.41
 C      -3.714253     2.677063    -1.645624      22.56
 O      -4.086084     3.865982    -1.241915     200.73
 C      -4.611754     3.855452     0.188688     102.55
 H      -5.366855     3.090152     0.315070      23.11
 H      -4.763696     5.019620     0.399954      24.75
 H      -3.709910     3.747067     0.709902      27.77
 C      -3.174399     2.597341    -3.002613       6.19
 O      -3.023469     3.593353    -3.808482     154.89
 H      -3.334579     4.510902    -3.403555      18.52
 C      -2.846463     1.300660    -3.589441      35.71
 H      -2.112630     1.499523    -4.432075      24.00
 C      -3.684192     0.274244    -1.535605      -8.28
 C      -3.873921    -1.136261    -0.860873      87.26
 H      -4.270711    -1.865083    -1.578246      26.33
 O      -4.601945    -1.112327     0.456606     214.21
 H      -4.026112    -0.824747     1.167048      27.92
 C      -2.492197    -1.886174    -0.598394      75.62
 H      -1.963817    -2.146527    -1.585541      24.44
 C      -2.803093    -3.312469     0.054113     102.84
 O      -3.746526    -4.117090    -0.656292     238.74
 H      -3.435243    -4.230081    -1.594519      28.70
 H      -3.216225    -3.203114     1.015164      26.15
 H      -1.655776    -3.859715     0.075919      21.29
 C       1.735665    -1.278148    -1.320410     104.92
 H       2.262222    -1.795690    -2.090585      21.16
 C       1.562279     0.428978     0.373072      21.37
 H       1.984175     1.235449     1.226278      19.67
 C       0.180305     0.164420     0.496764      -0.55
 O      -0.501605     0.740698     1.561364     234.72
 C      -0.614304     2.143319     1.254006     134.36
 H      -1.385848     2.694928     1.795801      26.92
 H       0.263960     2.673849     0.991921      26.46
 H      -1.469401     2.385467     0.503071      27.69
 C      -0.349837    -0.944378    -0.229620      16.29
 O      -1.636760    -1.000859     0.242520     170.25
 C       0.302697    -1.769452    -1.049117     106.79
 H       0.019357    -2.902503    -1.382708      18.53
 C       2.388738    -0.190211    -0.635354      31.25
 C       3.788695     0.263625    -1.098486     100.39
 H       3.976846     0.094385    -2.357365      21.90
 O       3.979198     1.671679    -0.991769     208.82
 H       4.413630     2.005204    -0.053421      22.61
 C       5.031991    -0.383200    -0.420394      92.54
 H       5.150930    -0.087676     0.646991      25.57
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 O       4.944017    -1.804966    -0.345643     275.72
 H       4.858400    -2.096184    -1.307520      29.27
 C       6.531483    -0.010453    -1.003005      95.54
 O       7.114400     1.283511    -0.757979     268.22
 H       7.201976     1.551397     0.208939      26.69
 H       6.488554    -0.285563    -1.918987      33.43
 H       7.046320    -0.876225    -0.405018      30.07
55
name= lig-ACN-Water-frame_513
 C      -3.152832     0.109222    -2.882967      57.38
 H      -3.246214    -0.858231    -3.383312      26.06
 C      -3.923606     1.416791    -1.008329      29.00
 H      -4.175843     1.335595     0.162713      22.28
 C      -3.705969     2.616487    -1.723010      17.07
 O      -4.146754     3.931643    -1.178421     191.97
 C      -4.616457     3.853218     0.168168     117.14
 H      -5.400544     3.105179     0.461010      27.88
 H      -5.296607     4.816313     0.323510      26.42
 H      -3.928284     3.683257     0.942294      30.46
 C      -3.202128     2.513189    -2.980653      15.90
 O      -3.040978     3.703855    -3.811449     151.59
 H      -3.343218     4.537450    -3.381171      25.08
 C      -2.851476     1.327891    -3.578830      83.94
 H      -2.544499     1.250937    -4.638331      20.62
 C      -3.616940     0.148499    -1.602388       2.59
 C      -3.898685    -1.112101    -0.808888      86.96
 H      -4.659515    -1.615512    -1.321012      25.22
 O      -4.624594    -1.048495     0.461026     180.69
 H      -4.002177    -0.793151     1.199811      25.81
 C      -2.514759    -2.013118    -0.572154      87.04
 H      -1.999305    -2.128655    -1.574997      24.23
 C      -2.743962    -3.315478     0.132626     112.25
 O      -3.686415    -4.138977    -0.630378     239.63
 H      -3.393612    -4.306592    -1.468813      31.72
 H      -3.162912    -3.120402     1.073405      27.65
 H      -1.766813    -4.075257     0.387991      24.22
 C       1.710010    -1.320405    -1.266033      44.93
 H       2.276021    -1.736902    -2.025061      24.88
 C       1.585998     0.415380     0.277465      45.78
 H       2.120947     1.017403     1.197647      23.64
 C       0.262649     0.141953     0.398721      -1.23
 O      -0.439469     0.733429     1.528302     177.70
 C      -0.776552     2.116721     1.311974     124.10
 H      -1.073649     2.290661     2.347583      25.77
 H       0.215999     2.518557     1.222060      26.26
 H      -1.097129     2.131797     0.205366      26.81
 C      -0.426568    -0.933236    -0.158751     -10.03
 O      -1.738503    -1.130998     0.213343     157.34
 C       0.483050    -1.730480    -1.060788      72.56
 H       0.022218    -2.474845    -1.930558      21.00
 C       2.312082    -0.175868    -0.698184      33.09
 C       3.741848     0.257603    -1.078197      86.04
 H       3.705356    -0.059777    -2.321593      24.49
 O       3.988969     1.726054    -0.989627     200.62
 H       4.351888     1.876513    -0.107986      27.40
 C       4.949383    -0.383267    -0.385354      88.57
 H       4.737673     0.063508     0.636221      25.53
 O       5.030491    -1.829673    -0.256300     256.12
 H       4.897559    -2.236593    -1.140108      29.04
 C       6.429412    -0.077461    -0.983132      91.33
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 O       7.076470     1.240817    -0.736638     217.03
 H       7.139229     1.476772     0.239744      25.89
 H       6.576297    -0.064471    -1.917108      28.88
 H       7.200115    -0.922058    -0.596511      27.73
55
name= lig-ACN-Water-frame_514
 C      -3.170216     0.073085    -2.939977      57.23
 H      -2.814872    -0.805475    -3.450856      24.64
 C      -3.914452     1.313993    -1.043970      70.87
 H      -3.931226     1.399225     0.101168      21.01
 C      -3.798377     2.612817    -1.668072       1.47
 O      -4.143556     3.873636    -1.162429     203.25
 C      -4.731099     3.888491     0.202895     107.32
 H      -5.262518     2.940693     0.111313      25.38
 H      -5.255082     4.893470     0.361547      24.87
 H      -3.896215     3.888157     0.926630      28.69
 C      -3.207272     2.658488    -3.071327      -6.52
 O      -3.036900     3.762529    -3.808776     141.62
 H      -3.484431     4.563648    -3.532324      24.02
 C      -2.896475     1.258949    -3.613989      31.68
 H      -2.752933     1.144215    -4.658777      22.01
 C      -3.591716     0.074219    -1.527696      22.69
 C      -3.932692    -1.285734    -0.740550     104.10
 H      -4.530449    -1.800051    -1.372999      27.83
 O      -4.614595    -0.935629     0.467815     221.53
 H      -3.992917    -0.525788     1.196503      22.17
 C      -2.676874    -2.060248    -0.657896      89.04
 H      -2.300506    -2.219401    -1.701002      25.37
 C      -2.736569    -3.381741     0.226856     108.41
 O      -3.660294    -4.187780    -0.529067     197.69
 H      -3.443952    -4.226527    -1.466066      29.74
 H      -3.196388    -3.196064     1.182371      26.25
 H      -1.519293    -3.678099     0.375719      24.18
 C       1.855356    -1.346927    -1.399091      52.95
 H       2.279162    -2.037085    -2.067556      19.44
 C       1.655034     0.506781     0.285287      43.71
 H       2.131640     1.524392     0.676313      22.11
 C       0.244007     0.081438     0.538797     -12.01
 O      -0.411504     0.643067     1.521717     207.86
 C      -0.814655     2.123054     1.361918     106.23
 H      -1.588287     2.487342     2.006325      25.99
 H       0.003943     2.922421     1.358054      25.16
 H      -1.716003     2.406112     0.651082      23.99
 C      -0.401671    -0.997723    -0.185108      14.67
 O      -1.729073    -1.254874     0.188009     162.87
 C       0.376309    -1.657055    -1.063638      59.00
 H      -0.137700    -2.510719    -1.753695      21.14
 C       2.390212    -0.213291    -0.734011      16.80
 C       3.730418     0.284183    -1.145960      82.81
 H       3.992970     0.149323    -2.385374      24.54
 O       3.938477     1.734342    -1.004369     217.83
 H       4.028868     2.013298    -0.133569      30.55
 C       5.020918    -0.423373    -0.307782      72.65
 H       5.110314    -0.109626     0.798973      27.57
 O       5.027935    -1.871113    -0.168600     213.50
 H       5.045275    -2.158366    -1.116667      29.57
 C       6.349962    -0.025542    -0.955715     103.72
 O       7.003384     1.196631    -0.707094     176.45
 H       7.314490     1.276705     0.231394      26.72
 H       6.100492    -0.197417    -1.866261      31.87
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 H       7.078361    -0.971880    -0.612923      29.24
55
name= lig-ACN-Water-frame_515
 C      -3.130389     0.024836    -2.923099      50.54
 H      -2.829500    -0.857789    -3.450503      23.31
 C      -3.855862     1.386021    -0.934768      35.14
 H      -4.527613     1.396989    -0.078662      18.22
 C      -3.795414     2.570234    -1.759279       7.77
 O      -4.108389     3.800945    -1.160858     198.18
 C      -4.809336     3.867186     0.173894     108.75
 H      -5.609139     3.249674     0.675143      25.04
 H      -5.299904     4.812399     0.118503      24.87
 H      -3.994778     3.877214     0.956742      27.09
 C      -3.300836     2.574790    -3.050655      10.84
 O      -3.013698     3.778967    -3.850196     206.72
 H      -3.364084     4.612970    -3.445918      20.73
 C      -3.037787     1.385456    -3.651284      49.59
 H      -2.369931     1.482811    -4.455621      24.46
 C      -3.616860    -0.001962    -1.612533      -0.51
 C      -3.992095    -1.266991    -0.777988      96.88
 H      -4.651130    -1.925497    -1.086757      26.79
 O      -4.619846    -0.870965     0.487597     216.23
 H      -3.919548    -0.650261     1.213441      21.15
 C      -2.666786    -2.139643    -0.563294      89.88
 H      -2.373726    -2.459406    -1.562265      24.47
 C      -2.783585    -3.345969     0.190763     111.36
 O      -3.657369    -4.350864    -0.395723     159.20
 H      -3.407662    -4.331719    -1.459054      27.09
 H      -3.054174    -3.172486     1.253805      24.97
 H      -1.715427    -4.018447     0.153729      22.08
 C       1.737155    -1.358191    -1.418937      46.81
 H       2.421603    -1.840147    -2.117558      21.85
 C       1.597937     0.480808     0.156469      54.90
 H       1.695332     1.536446     0.467159      19.84
 C       0.391181     0.021344     0.607624       2.39
 O      -0.537433     0.746476     1.659253     156.60
 C      -0.971803     2.104258     1.423695      93.22
 H      -1.349767     2.187788     2.392124      24.16
 H      -0.040851     2.846764     1.242764      22.78
 H      -1.386774     1.933494     0.306169      22.40
 C      -0.306742    -0.984157    -0.155899      -5.36
 O      -1.643156    -1.308386     0.147804     138.23
 C       0.423848    -1.689309    -1.229482      57.70
 H       0.027969    -2.718028    -1.488506      19.57
 C       2.435416    -0.252460    -0.765106      25.13
 C       3.919393     0.292730    -1.076296      71.83
 H       4.132257     0.002284    -2.259173      20.92
 O       3.862770     1.751358    -1.020119     222.37
 H       4.082345     1.973025    -0.036382      23.51
 C       5.037688    -0.407016    -0.197477      85.15
 H       4.876336     0.052331     0.881660      24.67
 O       4.975765    -1.895195    -0.137563     220.25
 H       4.911040    -2.210640    -1.104634      27.85
 C       6.334284    -0.077662    -0.980284      95.84
 O       6.943144     1.214788    -0.698134     222.89
 H       7.064708     1.389298     0.267736      29.24
 H       6.299623     0.019883    -1.957677      32.10
 H       7.190795    -0.976980    -0.812876      28.32
55
name= lig-ACN-Water-frame_516
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 C      -3.112465     0.154047    -2.955955      71.21
 H      -2.974266    -0.786802    -3.468444      24.60
 C      -3.905567     1.288475    -1.031104      84.81
 H      -4.388455     1.296080    -0.113290      20.77
 C      -3.792947     2.520825    -1.649973      10.88
 O      -4.144028     3.726846    -1.132925     226.61
 C      -4.830650     3.928213     0.119380     109.73
 H      -5.516597     3.076083    -0.006281      26.16
 H      -5.151795     4.895564     0.034459      26.06
 H      -4.144335     3.891539     1.114556      26.34
 C      -3.385396     2.597109    -3.089473      -4.94
 O      -3.013735     3.689370    -3.829823      64.88
 H      -3.320333     4.573082    -3.377441      20.49
 C      -3.023996     1.299474    -3.657115      42.45
 H      -2.566172     1.295779    -4.636002      22.17
 C      -3.715179     0.145012    -1.635760      38.13
 C      -3.963380    -1.186229    -0.746311      95.41
 H      -4.592685    -1.604426    -1.353011      25.82
 O      -4.617106    -0.850485     0.499022     241.53
 H      -3.990052    -0.650923     1.239989      22.73
 C      -2.570192    -2.061348    -0.595221      75.87
 H      -2.133876    -2.182734    -1.571219      23.05
 C      -2.778302    -3.522838     0.249715      85.19
 O      -3.719966    -4.514541    -0.301354     162.60
 H      -3.489281    -4.702691    -1.349249      27.15
 H      -3.234795    -3.328177     1.336665      23.51
 H      -1.587506    -3.859179     0.367534      22.61
 C       1.811467    -1.306636    -1.453215      43.34
 H       2.201267    -1.967710    -2.286636      21.26
 C       1.575011     0.505751     0.092845      19.01
 H       2.173537     1.248658     0.511335      20.42
 C       0.229761     0.022603     0.648943      -8.19
 O      -0.492654     0.686984     1.721034     190.74
 C      -1.045216     2.044326     1.384828      94.88
 H      -1.773682     2.506422     2.029434      23.97
 H      -0.102191     2.797984     1.334633      22.87
 H      -1.959396     2.264170     0.589519      20.31
 C      -0.263593    -1.076923    -0.179344       2.75
 O      -1.563444    -1.302627     0.164898     184.21
 C       0.443975    -1.728060    -1.204331      54.71
 H       0.036170    -2.434420    -1.874303      21.31
 C       2.407571    -0.241472    -0.789083      30.57
 C       3.849962     0.221897    -0.995705      85.65
 H       4.152563     0.035962    -2.125192      21.38
 O       3.860439     1.736691    -0.978760     186.39
 H       4.359031     2.153581    -0.094237      19.96
 C       5.051476    -0.402649    -0.228907      84.28
 H       5.201176    -0.066795     0.922484      22.74
 O       4.883021    -1.847759    -0.124096     264.14
 H       4.657002    -2.089099    -1.087646      26.51
 C       6.438575    -0.073766    -0.971277      86.01
 O       6.904213     1.272411    -0.673480     253.11
 H       6.912921     1.476183     0.305482      28.30
 H       6.176506    -0.192129    -1.919177      32.63
 H       7.279706    -0.983834    -0.709205      27.85
55
name= lig-ACN-Water-frame_517
 C      -3.211093     0.101919    -2.947937      53.69
 H      -2.832694    -0.811901    -3.443854      23.36
 C      -4.090988     1.368819    -0.980260      39.11
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 H      -3.989340     1.366885     0.028915      20.48
 C      -3.793738     2.568257    -1.713127       7.66
 O      -4.094092     3.788580    -1.142870     237.01
 C      -4.892963     3.921996     0.037437     102.85
 H      -5.864465     3.363094     0.291689      26.93
 H      -5.267939     4.851687     0.092987      27.00
 H      -4.201356     3.603683     0.973071      26.69
 C      -3.359177     2.499071    -3.050730      12.83
 O      -3.056906     3.639799    -3.775101     176.77
 H      -3.556489     4.515913    -3.450172      21.38
 C      -2.971063     1.347286    -3.693934      60.83
 H      -2.935990     1.232015    -4.797567      22.94
 C      -3.660518     0.065760    -1.647356      16.79
 C      -3.824232    -1.116971    -0.784506     114.29
 H      -4.362177    -1.850855    -1.121331      29.29
 O      -4.596080    -0.870207     0.481505     201.48
 H      -4.004114    -0.588225     1.198606      25.02
 C      -2.571979    -2.026388    -0.604601      86.11
 H      -2.295864    -2.355538    -1.603820      25.21
 C      -2.779677    -3.606361     0.240840      86.17
 O      -3.718638    -4.625106    -0.253142     204.13
 H      -3.452413    -4.814366    -1.112360      33.28
 H      -3.305784    -3.120003     1.244748      23.67
 H      -1.770263    -4.198322     0.517403      23.52
 C       1.839410    -1.347922    -1.543933      34.01
 H       2.564857    -1.736421    -2.339518      15.73
 C       1.525554     0.489873     0.270286      67.99
 H       1.836131     1.200719     0.911885      21.74
 C       0.263695     0.098641     0.504133     -11.62
 O      -0.448297     0.595009     1.664999     131.89
 C      -1.120102     2.029237     1.357445      77.08
 H      -1.552591     2.178496     2.361688      22.67
 H      -0.306940     2.860293     1.065145      22.57
 H      -1.560750     1.643757     0.253502      19.85
 C      -0.287178    -1.070518    -0.124169      -2.05
 O      -1.634234    -1.328017     0.240921     163.03
 C       0.506025    -1.708158    -1.157187      72.64
 H      -0.039524    -2.193241    -1.832976      23.57
 C       2.311743    -0.221214    -0.749769       2.41
 C       3.759301     0.286709    -1.002473      81.57
 H       3.900842     0.002991    -2.109823      21.12
 O       3.910791     1.701521    -0.927832     223.59
 H       4.315742     1.875640     0.062972      18.34
 C       5.118139    -0.422784    -0.244425      66.06
 H       5.118829     0.015640     0.905179      23.07
 O       4.784040    -1.794085    -0.153139     307.28
 H       4.723988    -2.138929    -1.076962      29.77
 C       6.451084    -0.045763    -0.911819     103.80
 O       6.873037     1.328732    -0.689353     235.16
 H       7.098869     1.410716     0.280757      30.49
 H       6.591947    -0.127353    -1.885916      32.15
 H       7.346489    -0.750775    -0.322437      27.24
55
name= lig-ACN-Water-frame_518
 C      -3.242161     0.027593    -2.984405      60.28
 H      -3.036110    -0.994249    -3.411838      22.77
 C      -4.053004     1.374078    -0.993885      69.05
 H      -4.590415     1.487539    -0.072187      19.62
 C      -3.893123     2.555940    -1.712796       4.88
 O      -4.044719     3.899630    -1.220951     191.37
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 C      -4.966639     3.914750     0.047434      97.19
 H      -5.803431     3.248804    -0.239730      24.39
 H      -4.975146     4.927775     0.144678      25.26
 H      -4.300471     3.597559     1.066374      22.93
 C      -3.266033     2.517643    -3.028007     -13.80
 O      -3.131727     3.683129    -3.750788     137.47
 H      -3.567398     4.450849    -3.234149      17.97
 C      -3.062482     1.222925    -3.664092      33.72
 H      -2.484295     1.442153    -4.644083      23.26
 C      -3.658492     0.155763    -1.572595       3.59
 C      -3.821850    -1.296414    -0.749091      98.14
 H      -4.467928    -1.702324    -1.366994      28.99
 O      -4.517403    -0.899822     0.432509     241.95
 H      -3.849797    -0.686501     1.145040      24.16
 C      -2.575400    -2.187494    -0.541603      95.70
 H      -2.010849    -2.228297    -1.482867      24.54
 C      -2.850708    -3.499047     0.202177     100.70
 O      -3.671890    -4.648087    -0.233237     212.47
 H      -3.458586    -4.835527    -1.161723      31.59
 H      -3.214787    -3.379172     1.438986      22.92
 H      -1.754700    -3.777807     0.198256      24.83
 C       1.747254    -1.206992    -1.398512      42.33
 H       2.235169    -1.705871    -2.275840      20.25
 C       1.601265     0.426758     0.377786      58.76
 H       2.014040     1.227695     0.880849      20.30
 C       0.221702     0.061897     0.526391       1.11
 O      -0.414446     0.636886     1.554810     230.19
 C      -1.076796     1.818819     1.304695     113.08
 H      -1.791745     2.132859     2.066169      24.55
 H      -0.311868     2.740273     1.160270      22.82
 H      -2.085245     1.847946     0.478196      21.72
 C      -0.309706    -1.047868    -0.169753     -16.29
 O      -1.648930    -1.380622     0.282152     140.05
 C       0.456564    -1.709023    -1.196088      66.14
 H       0.151242    -2.625433    -1.475482      22.59
 C       2.368997    -0.153599    -0.659755      17.25
 C       3.804846     0.305329    -1.039981      99.95
 H       3.953519     0.139616    -2.142739      23.72
 O       3.943997     1.714454    -0.902482     250.51
 H       4.053460     2.086825     0.087108      19.16
 C       4.941476    -0.353062    -0.312638      75.07
 H       4.960839     0.060616     0.845840      23.33
 O       4.769519    -1.810431    -0.208072     281.77
 H       4.870532    -2.110881    -1.147826      28.82
 C       6.514177    -0.027947    -0.831008      81.19
 O       6.857007     1.405550    -0.700803     241.70
 H       6.817592     1.761859     0.241591      28.14
 H       6.605345    -0.341420    -1.783962      31.25
 H       7.262610    -0.838421    -0.169490      27.88
55
name= lig-ACN-Water-frame_519
 C      -3.270998     0.032306    -2.862540      47.91
 H      -3.187714    -0.927834    -3.436634      22.64
 C      -4.010788     1.361837    -1.006310      29.25
 H      -4.732824     1.102957    -0.190527      17.52
 C      -3.879520     2.623714    -1.732602      12.76
 O      -4.080182     3.887591    -1.222513     220.21
 C      -4.882993     3.982201    -0.052477     122.02
 H      -5.888226     3.476973    -0.169118      24.80
 H      -5.396683     4.916253     0.187061      23.97
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 H      -4.435809     3.295022     0.883040      23.45
 C      -3.291765     2.524172    -3.027781       9.45
 O      -3.176722     3.713647    -3.737215     201.85
 H      -3.343404     4.542122    -3.280407      23.08
 C      -3.076617     1.246784    -3.633470      51.87
 H      -2.512167     0.947810    -4.598009      23.41
 C      -3.634518     0.036344    -1.567889      26.64
 C      -3.916523    -1.267361    -0.843488     100.46
 H      -4.551897    -1.940141    -1.285810      28.35
 O      -4.473015    -1.009347     0.446848     193.14
 H      -3.805692    -0.584997     1.131450      21.29
 C      -2.616749    -2.200771    -0.576572      81.97
 H      -2.249701    -2.647853    -1.545267      24.39
 C      -2.768183    -3.514248     0.242760      98.56
 O      -3.617978    -4.568600    -0.260357     182.96
 H      -3.497497    -4.657343    -1.360999      26.57
 H      -3.257473    -3.129359     1.400080      22.43
 H      -1.801673    -3.992163     0.433771      25.48
 C       1.692951    -1.103995    -1.315786      41.82
 H       2.333214    -1.622772    -2.026604      22.08
 C       1.689799     0.403680     0.395691      36.58
 H       2.022573     1.154942     1.159521      21.08
 C       0.328705    -0.014544     0.557193     -25.81
 O      -0.448144     0.613976     1.583604     208.88
 C      -1.180940     1.847582     1.247472      81.85
 H      -1.546711     2.060613     2.221593      24.82
 H      -0.336606     2.642232     0.901761      24.40
 H      -1.805696     1.662658     0.099645      22.80
 C      -0.436113    -1.068328    -0.229113      -3.43
 O      -1.600088    -1.456166     0.325786     149.31
 C       0.353397    -1.704369    -1.108895      65.09
 H       0.297140    -2.650747    -1.635518      23.33
 C       2.433536    -0.160634    -0.629979      16.90
 C       3.806356     0.354206    -1.112813      97.79
 H       3.883269     0.126409    -2.167535      24.41
 O       3.929742     1.810597    -0.955618     228.49
 H       4.264261     2.083179    -0.059004      23.18
 C       4.944564    -0.370833    -0.298413      81.08
 H       4.683319    -0.062891     0.874706      23.69
 O       4.806244    -1.806945    -0.292443     284.98
 H       4.776870    -2.101211    -1.271902      26.03
 C       6.419512     0.033885    -0.716946      91.16
 O       6.856413     1.429445    -0.740585     246.80
 H       6.699492     1.659726     0.206220      29.01
 H       6.582595    -0.301358    -1.700015      29.65
 H       7.178198    -0.559893     0.111967      26.19
55
name= lig-ACN-Water-frame_520
 C      -3.237448     0.069617    -2.907320      59.21
 H      -2.970831    -0.857363    -3.443868      23.09
 C      -4.049935     1.291263    -1.005410      67.33
 H      -4.218636     1.620564     0.095906      20.16
 C      -3.795235     2.506297    -1.678068       1.76
 O      -4.125074     3.853089    -1.255620     218.47
 C      -4.936557     3.976853    -0.068040      90.47
 H      -5.856308     3.335605    -0.117078      27.84
 H      -4.718494     5.081326     0.009041      24.41
 H      -4.185435     3.744274     0.904119      25.40
 C      -3.370999     2.550928    -3.063103      -4.12
 O      -3.150976     3.707821    -3.793090     154.98
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 H      -3.624363     4.419796    -3.318147      23.41
 C      -3.031030     1.290401    -3.576996      52.80
 H      -2.999684     1.369978    -4.701936      23.25
 C      -3.696507     0.054655    -1.551487      31.91
 C      -3.907372    -1.313701    -0.789038      97.66
 H      -4.620633    -1.821608    -1.396685      25.91
 O      -4.527269    -1.141448     0.501677     227.05
 H      -3.899381    -0.633909     1.150917      22.28
 C      -2.608540    -2.199945    -0.628599      79.39
 H      -2.052438    -2.216715    -1.627764      22.40
 C      -2.712329    -3.548831     0.342252      89.54
 O      -3.612414    -4.455659    -0.342121     196.02
 H      -3.317881    -4.389699    -1.321305      28.18
 H      -3.377564    -3.224557     1.424310      21.37
 H      -1.728201    -3.841990     0.550283      25.38
 C       1.734662    -1.232684    -1.410722      46.06
 H       2.222291    -1.710803    -2.226097      22.31
 C       1.641706     0.399370     0.483527      35.47
 H       2.025258     1.220971     1.280968      22.26
 C       0.297843    -0.033831     0.638267      33.76
 O      -0.455218     0.515021     1.650675     132.19
 C      -1.177526     1.948139     1.146495      62.00
 H      -1.834718     2.313510     1.864464      26.33
 H      -0.452260     2.812811     0.797717      24.25
 H      -2.087685     1.467803     0.389457      19.95
 C      -0.371727    -0.976074    -0.097577     -39.82
 O      -1.667059    -1.538769     0.283762     140.79
 C       0.479680    -1.684419    -1.128501      55.02
 H      -0.251987    -2.233179    -1.846533      19.47
 C       2.388967    -0.125881    -0.646478     -11.07
 C       3.790660     0.396273    -1.108211      98.59
 H       3.949743     0.177723    -2.113850      26.23
 O       3.889693     1.868701    -1.098813     246.76
 H       4.123539     2.090519    -0.210248      27.89
 C       4.955417    -0.357162    -0.249016      82.98
 H       4.816018    -0.102103     0.933317      25.09
 O       4.856329    -1.792487    -0.394425     254.51
 H       4.943040    -2.042897    -1.407031      26.22
 C       6.363913     0.066232    -0.627303      99.12
 O       6.807300     1.449555    -0.747695     212.51
 H       7.208199     1.792702     0.066281      28.25
 H       6.622721    -0.448366    -1.573973      30.60
 H       7.131162    -0.533870     0.152518      26.96
55
name= lig-ACN-Water-frame_521
 C      -3.187468     0.095638    -2.927301      62.56
 H      -2.911137    -0.832470    -3.412502      23.06
 C      -4.020771     1.347804    -0.914686      60.41
 H      -4.218945     1.155468     0.243060      18.64
 C      -3.796883     2.509843    -1.664842      28.87
 O      -4.148867     3.717418    -1.304434     198.37
 C      -4.857563     4.037985     0.010912      96.47
 H      -5.886126     3.537941     0.049227      28.65
 H      -5.476230     5.063174    -0.024418      25.43
 H      -4.318835     3.620481     1.009011      27.89
 C      -3.371734     2.534225    -3.059115      18.42
 O      -3.162876     3.683975    -3.830755     127.04
 H      -3.680780     4.558746    -3.610917      18.01
 C      -3.051620     1.323459    -3.662743      50.50
 H      -2.528125     1.286519    -4.646272      24.91
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 C      -3.735334     0.069694    -1.565319      21.72
 C      -3.882386    -1.374590    -0.689209      94.92
 H      -4.542179    -1.988726    -1.352615      24.69
 O      -4.611150    -1.261518     0.539784     213.93
 H      -4.031191    -0.960238     1.272696      24.65
 C      -2.523005    -2.206759    -0.530469      98.24
 H      -2.224539    -2.616629    -1.578331      23.14
 C      -2.765720    -3.449933     0.226866     107.48
 O      -3.607221    -4.391865    -0.439698     244.71
 H      -3.315756    -4.537345    -1.265255      34.01
 H      -3.216487    -3.178407     1.395011      23.36
 H      -1.846020    -3.943220     0.357608      26.41
 C       1.859309    -1.248698    -1.465127      39.40
 H       2.286760    -1.552777    -2.385222      19.29
 C       1.576587     0.333886     0.435467      47.34
 H       2.181656     1.300696     0.934272      21.93
 C       0.236296    -0.008497     0.788572     -19.71
 O      -0.554661     0.648498     1.770185     170.96
 C      -1.185605     1.871323     1.133452      84.93
 H      -1.534882     2.380689     1.917962      26.96
 H      -0.194657     2.393914     0.685016      23.97
 H      -1.763242     1.703523     0.042106      21.05
 C      -0.269921    -1.138589    -0.076343       6.96
 O      -1.587739    -1.422351     0.250575     142.44
 C       0.428102    -1.568333    -1.141456      53.47
 H       0.059389    -2.428285    -1.927515      20.51
 C       2.307711    -0.162024    -0.696519      15.65
 C       3.757554     0.370969    -1.042939      83.45
 H       3.919258     0.003222    -1.983657      27.93
 O       3.830897     1.891016    -1.181299     199.69
 H       4.154602     2.350681    -0.367398      26.74
 C       4.886972    -0.275330    -0.247114      82.94
 H       4.695486    -0.181375     0.912954      25.41
 O       4.904586    -1.754049    -0.466420     272.07
 H       4.973304    -1.936418    -1.494721      27.47
 C       6.461424     0.051696    -0.605934      86.00
 O       6.762768     1.479554    -0.728109     208.74
 H       7.025267     1.652018     0.230476      27.27
 H       6.599728    -0.415772    -1.621959      31.34
 H       7.104129    -0.489901     0.249726      28.06
55
name= lig-ACN-Water-frame_522
 C      -3.203246     0.087895    -2.841698      61.59
 H      -2.927830    -0.827684    -3.316131      23.38
 C      -3.925150     1.241170    -0.894680      66.07
 H      -4.647356     1.412657     0.010480      19.62
 C      -3.894884     2.475587    -1.659258      -5.17
 O      -4.231510     3.816483    -1.185209     222.09
 C      -4.884011     3.994920    -0.000073      88.56
 H      -5.589038     3.093214     0.197031      23.14
 H      -5.011697     5.192117    -0.071672      22.14
 H      -4.030768     4.069739     0.838116      24.79
 C      -3.331155     2.490535    -3.113652      -3.34
 O      -3.199226     3.669373    -3.853404     152.52
 H      -3.587627     4.425746    -3.194808      18.92
 C      -3.027192     1.248744    -3.710017      58.65
 H      -2.409939     1.184468    -4.604444      24.22
 C      -3.673371     0.016539    -1.548111      40.16
 C      -3.845118    -1.328320    -0.742901      94.03
 H      -4.389632    -2.173066    -1.254448      22.74
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 O      -4.627162    -1.348015     0.578039     204.71
 H      -4.117390    -0.823290     1.211718      24.77
 C      -2.520400    -2.100593    -0.515286      80.95
 H      -1.993372    -2.233441    -1.550460      21.45
 C      -2.734151    -3.494858     0.182467      97.78
 O      -3.684480    -4.361645    -0.526621     191.18
 H      -3.297417    -4.577666    -1.481947      26.60
 H      -3.399946    -3.318909     1.214481      22.78
 H      -1.774992    -3.902711     0.422170      25.83
 C       1.739601    -1.160318    -1.478711      40.30
 H       2.396063    -1.595744    -2.210370      21.80
 C       1.535249     0.354354     0.360264      31.64
 H       1.922902     1.356487     1.018959      20.64
 C       0.306502    -0.120425     0.794196      -4.29
 O      -0.636258     0.727911     1.830355      94.34
 C      -1.023681     1.859507     1.108479     117.13
 H      -1.601797     2.520177     1.709154      28.06
 H      -0.159434     2.552266     0.638259      24.10
 H      -1.984698     1.486606     0.407809      22.94
 C      -0.208099    -1.131100     0.018080     -22.72
 O      -1.526152    -1.289949     0.239582     109.91
 C       0.507950    -1.614456    -1.254750      61.34
 H       0.003836    -2.611961    -1.718745      18.96
 C       2.362611    -0.164801    -0.654107      35.77
 C       3.704156     0.384311    -1.083516      91.54
 H       3.861640     0.158888    -2.076132      25.62
 O       3.752624     1.854867    -1.187380     177.97
 H       4.420710     2.006632    -0.382583      22.54
 C       4.972508    -0.303257    -0.237448      93.88
 H       4.761080    -0.113464     0.860584      24.38
 O       4.903324    -1.685501    -0.487453     319.10
 H       4.922273    -1.896318    -1.475901      27.33
 C       6.389398     0.100271    -0.614547     103.15
 O       6.761888     1.477329    -0.651559     294.81
 H       6.587624     1.941808     0.216098      29.66
 H       6.786531    -0.302913    -1.614130      27.88
 H       7.145289    -0.441424     0.087037      27.44
55
name= lig-ACN-Water-frame_523
 C      -3.170574    -0.038511    -2.868198      48.46
 H      -2.948027    -0.980251    -3.338548      24.72
 C      -3.991255     1.303383    -0.968884      66.70
 H      -4.321747     1.256182     0.113841      22.40
 C      -3.905214     2.468673    -1.763642      24.08
 O      -4.221621     3.797438    -1.260435     206.90
 C      -4.849325     3.997143     0.132086      94.99
 H      -5.724231     3.306635     0.496047      25.34
 H      -5.649877     4.898345     0.098294      25.34
 H      -4.022137     3.975278     0.946782      26.26
 C      -3.377821     2.459466    -3.034591       8.69
 O      -3.248365     3.637196    -3.792925     155.16
 H      -3.608291     4.509956    -3.355321      22.67
 C      -2.987017     1.167377    -3.569618      45.41
 H      -2.922632     1.122179    -4.647100      23.72
 C      -3.637861     0.002817    -1.441760      -6.69
 C      -3.835109    -1.347472    -0.726278      90.40
 H      -4.467746    -1.767065    -1.576160      22.47
 O      -4.541161    -1.333787     0.521864     203.36
 H      -4.127740    -0.687860     1.179159      24.92
 C      -2.435440    -2.002238    -0.581435      80.74
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 H      -2.042361    -2.082389    -1.657888      24.13
 C      -2.729878    -3.534086     0.160539      93.71
 O      -3.727125    -4.335043    -0.608918     154.16
 H      -3.387119    -4.370617    -1.657792      25.28
 H      -3.221878    -3.264449     1.219983      23.70
 H      -1.810117    -4.104503     0.254969      25.48
 C       1.748848    -1.113192    -1.487202      31.40
 H       2.223626    -1.590907    -2.371571      20.96
 C       1.603622     0.503437     0.441764      15.35
 H       2.040297     1.495153     1.045888      18.53
 C       0.373221    -0.113572     0.835059       2.42
 O      -0.463711     0.610974     1.760505     111.45
 C      -1.013598     1.978720     1.062703      76.33
 H      -1.445644     2.508281     1.914951      26.10
 H      -0.099611     2.549998     0.489735      24.60
 H      -1.667252     1.641901     0.121872      24.14
 C      -0.246876    -1.121008    -0.089719     -10.98
 O      -1.617419    -1.237870     0.290456     151.76
 C       0.435455    -1.727788    -1.098143      67.69
 H      -0.051631    -2.418429    -1.894987      21.76
 C       2.354104    -0.120030    -0.636550       8.40
 C       3.762681     0.362922    -1.155306      85.43
 H       3.830333    -0.075960    -2.129288      24.46
 O       3.727689     1.816804    -1.102265     249.86
 H       4.272092     2.227090    -0.377434      21.53
 C       4.941795    -0.264878    -0.322626      99.64
 H       4.843645    -0.105506     0.752872      25.24
 O       4.863695    -1.713260    -0.475060     298.87
 H       5.148944    -1.891254    -1.387429      29.17
 C       6.414247     0.137910    -0.643970      92.21
 O       6.732908     1.553195    -0.585245     306.51
 H       6.777602     1.750141     0.396787      28.66
 H       6.477466    -0.190420    -1.751120      29.57
 H       6.985169    -0.510909     0.072625      29.39
55
name= lig-ACN-Water-frame_524
 C      -3.159653    -0.106623    -2.763848      62.92
 H      -3.049617    -1.039136    -3.312105      23.90
 C      -4.067533     1.305958    -0.980593      70.80
 H      -4.179618     1.482970     0.051542      24.40
 C      -3.926891     2.526783    -1.680241      15.72
 O      -4.254538     3.741393    -1.285208     157.57
 C      -4.870629     3.949349     0.200173      99.75
 H      -5.271707     2.878898     0.274678      23.75
 H      -5.322264     5.003017     0.036492      24.57
 H      -4.032122     4.121982     0.892970      29.11
 C      -3.412152     2.419916    -3.002031      12.08
 O      -3.279398     3.570941    -3.754370      64.81
 H      -3.759810     4.302667    -3.312351      23.61
 C      -3.060418     1.153879    -3.498436      51.79
 H      -2.721348     1.071961    -4.551309      24.12
 C      -3.588351     0.062816    -1.513091      22.47
 C      -3.783007    -1.279264    -0.768370      73.56
 H      -4.411083    -2.149924    -1.203736      22.02
 O      -4.499342    -1.272160     0.453608     187.79
 H      -3.892265    -0.900888     1.220760      23.56
 C      -2.485640    -2.166924    -0.591391      79.97
 H      -1.900833    -2.344716    -1.522504      24.40
 C      -2.720458    -3.456452     0.003820     118.57
 O      -3.735017    -4.270083    -0.670361     215.86
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 H      -3.609265    -4.188470    -1.621769      28.73
 H      -3.136290    -3.351846     1.055089      25.73
 H      -1.756291    -4.115563     0.132748      25.20
 C       1.683161    -1.166082    -1.341795      47.98
 H       2.191427    -1.329625    -2.333478      20.61
 C       1.721991     0.464266     0.462762      41.63
 H       2.188286     1.373347     1.073184      18.67
 C       0.430353    -0.006144     0.710181      11.17
 O      -0.311533     0.580731     1.643244     167.54
 C      -0.919148     1.990526     1.028241      84.07
 H      -1.405737     2.388932     2.035086      25.29
 H       0.102473     2.440396     0.915080      24.44
 H      -1.758395     1.859164     0.283451      24.97
 C      -0.336424    -1.009797     0.009210     -19.20
 O      -1.651810    -1.232242     0.298153      91.51
 C       0.460115    -1.704429    -1.022705      76.64
 H      -0.005527    -2.360586    -1.744036      25.60
 C       2.337375    -0.086749    -0.705413      10.03
 C       3.748032     0.349456    -1.134157     103.18
 H       3.960386     0.239835    -2.211338      24.15
 O       3.745283     1.828786    -1.052874     258.40
 H       4.218000     1.998114    -0.246318      23.03
 C       4.889120    -0.261746    -0.340011      90.93
 H       4.596881    -0.032555     0.638439      26.77
 O       4.842110    -1.760977    -0.465612     325.22
 H       5.103063    -2.049458    -1.363850      29.52
 C       6.389352     0.182051    -0.733383     105.12
 O       6.694074     1.598207    -0.502186     326.03
 H       7.051204     1.741336     0.402489      30.18
 H       6.722603    -0.004693    -1.841144      28.56
 H       7.152002    -0.407370    -0.265120      29.13
55
name= lig-ACN-Water-frame_525
 C      -3.152927     0.024016    -2.818061      57.14
 H      -2.819579    -0.971527    -3.173423      22.03
 C      -4.040674     1.256424    -0.859756      69.45
 H      -4.568082     1.147391    -0.016537      20.03
 C      -3.934404     2.445129    -1.625540       8.27
 O      -4.334428     3.801824    -1.175825     237.56
 C      -4.775535     3.854019     0.076043     140.85
 H      -5.636932     3.258623     0.556455      24.26
 H      -5.512719     4.713703     0.147195      25.30
 H      -3.942482     3.938390     0.749027      27.44
 C      -3.445029     2.374173    -2.987500       5.85
 O      -3.308440     3.506117    -3.754915     166.59
 H      -3.590825     4.361883    -3.321002      19.76
 C      -3.104161     1.119674    -3.587612      63.03
 H      -2.478609     1.226282    -4.527074      26.96
 C      -3.666329     0.018307    -1.442759      21.06
 C      -3.758346    -1.351883    -0.815866      91.44
 H      -4.430976    -1.673675    -1.715156      23.50
 O      -4.499399    -1.180633     0.462622     190.63
 H      -3.897306    -0.738368     1.179142      22.96
 C      -2.476614    -2.074112    -0.646053      83.87
 H      -2.018728    -2.161077    -1.624954      25.86
 C      -2.731127    -3.548145     0.004373     107.05
 O      -3.771591    -4.195461    -0.756970     229.22
 H      -3.554987    -4.200554    -1.636857      32.18
 H      -3.095541    -3.441923     1.034587      26.02
 H      -1.630955    -3.950851    -0.122177      23.91
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 C       1.711255    -1.185426    -1.326495      51.47
 H       2.105842    -1.923493    -2.093125      21.31
 C       1.785666     0.346033     0.414935      51.56
 H       2.236203     1.044874     1.113080      23.10
 C       0.422507     0.066917     0.581090     -43.10
 O      -0.328171     0.749308     1.633384     199.01
 C      -0.742544     1.935272     1.192134     126.36
 H      -1.523406     2.479432     1.962811      25.23
 H      -0.182549     2.780165     0.777482      26.94
 H      -1.308367     1.715140     0.253172      29.87
 C      -0.264344    -1.009009     0.008007      13.73
 O      -1.644750    -1.283171     0.304769     122.68
 C       0.395723    -1.626439    -0.973388      62.84
 H       0.074876    -2.505688    -1.301898      25.22
 C       2.421241    -0.129001    -0.751611      17.38
 C       3.687163     0.434113    -1.201279      76.93
 H       3.746103     0.061431    -2.299282      23.74
 O       3.802517     1.859223    -0.993387     217.72
 H       4.196026     2.199940    -0.114434      21.66
 C       4.935419    -0.365492    -0.351686      76.93
 H       4.999462    -0.199542     0.642419      27.46
 O       4.831482    -1.763958    -0.448072     303.94
 H       4.922639    -1.942870    -1.451287      27.49
 C       6.356226     0.254913    -0.797029      91.73
 O       6.660510     1.613220    -0.447838     298.52
 H       6.689392     1.727632     0.544109      28.41
 H       6.289418     0.221907    -1.976663      27.61
 H       6.934390    -0.451366    -0.318164      30.69
55
name= lig-ACN-Water-frame_526
 C      -3.157962     0.035483    -2.803830      55.09
 H      -2.650010    -0.846267    -3.236593      26.69
 C      -4.057816     1.207524    -0.766285      68.97
 H      -4.564725     1.206640     0.114708      19.77
 C      -3.965140     2.423894    -1.599442       5.36
 O      -4.343943     3.685154    -1.265641     184.11
 C      -4.831154     3.873789     0.213382     107.25
 H      -5.392542     2.940867     0.236444      24.30
 H      -5.102557     4.920164     0.271921      26.02
 H      -4.065811     3.687158     0.933676      29.09
 C      -3.496349     2.396223    -2.960395      11.79
 O      -3.336808     3.490800    -3.781425     107.65
 H      -3.635633     4.426735    -3.365353      20.17
 C      -3.087150     1.238925    -3.644973      28.20
 H      -2.843803     1.177409    -4.779204      23.65
 C      -3.644260     0.041667    -1.508200      27.63
 C      -3.890439    -1.275581    -0.784799      83.27
 H      -4.488781    -2.277967    -1.144957      20.57
 O      -4.539642    -1.158349     0.427207     159.87
 H      -4.005288    -0.659355     1.069824      28.28
 C      -2.433930    -2.024295    -0.633585      75.16
 H      -1.935686    -2.065325    -1.562149      28.32
 C      -2.737676    -3.509810    -0.039125     102.64
 O      -3.805751    -4.157756    -0.818247     162.67
 H      -3.494306    -4.303259    -1.805769      25.46
 H      -3.064460    -3.417912     0.946323      28.72
 H      -1.944596    -4.454368     0.134849      25.22
 C       1.772417    -1.336075    -1.462894      37.29
 H       2.463148    -1.921308    -2.125965      18.24
 C       1.735102     0.340178     0.396259      45.63
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 H       2.221075     1.029246     0.949852      25.09
 C       0.331507     0.124508     0.721857       0.24
 O      -0.215740     0.790011     1.729948     226.34
 C      -0.761411     2.144034     1.171075      92.14
 H      -1.492227     2.465265     2.134166      25.75
 H       0.113882     2.625882     1.190394      28.56
 H      -1.397992     2.054817     0.271368      29.96
 C      -0.333871    -0.952984    -0.027267      -7.86
 O      -1.589272    -1.321266     0.331340     161.62
 C       0.459923    -1.708790    -1.013026      66.73
 H       0.127695    -2.547837    -1.407428      28.03
 C       2.396353    -0.240107    -0.746328       4.18
 C       3.823571     0.399540    -1.137965      71.50
 H       4.074574     0.437745    -2.301754      25.15
 O       3.846513     1.913678    -0.992994     159.18
 H       4.046882     1.950569     0.047756      25.80
 C       4.945528    -0.289397    -0.387059     110.42
 H       4.653974    -0.077820     0.529689      31.58
 O       4.842326    -1.778302    -0.500530     293.05
 H       5.043300    -2.153112    -1.441743      27.04
 C       6.298646     0.226337    -0.868445      98.90
 O       6.606025     1.627469    -0.398789     211.47
 H       6.787395     1.602879     0.601781      27.20
 H       6.395504     0.336042    -2.085121      27.98
 H       7.140502    -0.306699    -0.783527      32.40
55
name= lig-ACN-Water-frame_527
 C      -3.116380     0.044404    -2.865172      70.14
 H      -3.030753    -0.936668    -3.372730      22.86
 C      -4.064710     1.240087    -0.910819      90.21
 H      -4.191486     1.281681     0.173880      24.40
 C      -3.968962     2.393405    -1.632059      18.76
 O      -4.365148     3.650248    -1.213176     187.41
 C      -4.834355     3.803229     0.229829     126.01
 H      -5.868975     3.519911     0.539809      26.07
 H      -5.073968     4.793492     0.294840      29.19
 H      -4.007089     3.550767     0.816097      28.41
 C      -3.515270     2.439312    -2.993175      15.03
 O      -3.391469     3.569924    -3.802861      18.68
 H      -3.928672     4.412017    -3.381924      19.28
 C      -3.131023     1.219670    -3.534860      49.49
 H      -2.959877     1.299385    -4.671236      25.59
 C      -3.681510     0.023042    -1.532500       9.23
 C      -3.826004    -1.308885    -0.764105      71.70
 H      -4.543067    -1.886755    -1.646907      23.50
 O      -4.644994    -1.133819     0.492392     147.87
 H      -4.098643    -0.815354     1.226949      25.48
 C      -2.458687    -2.099951    -0.563719      92.25
 H      -2.018993    -2.113448    -1.520658      26.49
 C      -2.803767    -3.452760    -0.084394     112.97
 O      -3.849404    -4.130837    -0.830793     109.58
 H      -3.527827    -4.180817    -1.912983      23.11
 H      -3.320885    -3.235515     0.780706      26.75
 H      -1.675636    -3.935408    -0.039504      23.80
 C       1.832258    -1.393086    -1.438129      46.98
 H       2.189760    -1.826528    -2.382551      21.29
 C       1.648070     0.374957     0.303596      46.71
 H       2.050072     1.149065     0.736088      24.50
 C       0.407754    -0.007452     0.727534      23.98
 O      -0.214531     0.858320     1.840755      83.72
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 C      -0.764251     2.311930     1.257487      84.84
 H      -1.510586     2.793512     2.166832      25.27
 H      -0.028696     2.968962     1.160678      29.18
 H      -1.144520     2.362379     0.282449      29.25
 C      -0.230106    -0.937555    -0.114036     -39.82
 O      -1.586888    -1.342325     0.378238     107.59
 C       0.531544    -1.777915    -1.061189      63.09
 H      -0.105323    -2.418860    -1.586722      24.24
 C       2.406537    -0.282110    -0.739181       9.39
 C       3.788241     0.391531    -1.148642      67.55
 H       3.898941     0.058476    -2.345801      23.39
 O       3.874612     1.867056    -0.946320     214.64
 H       4.106230     2.191184     0.001650      23.13
 C       4.966335    -0.302198    -0.384711     101.46
 H       5.062516    -0.124226     0.572027      30.47
 O       4.876867    -1.745025    -0.545747     301.25
 H       5.110600    -1.863694    -1.535562      28.47
 C       6.369849     0.282692    -0.931408      92.33
 O       6.566443     1.585549    -0.368011     229.22
 H       7.004821     1.501177     0.512948      30.63
 H       6.094493     0.471499    -2.113598      30.21
 H       6.978413    -0.440667    -0.683960      34.03
55
name= lig-ACN-Water-frame_528
 C      -3.214627    -0.045706    -2.849206      52.75
 H      -3.032383    -0.953122    -3.464208      18.78
 C      -4.007143     1.238094    -1.025318      60.59
 H      -4.417364     1.220608     0.093578      18.76
 C      -4.000910     2.508567    -1.718714      32.23
 O      -4.441801     3.667882    -1.076341     242.50
 C      -4.824327     3.821772     0.197102     138.22
 H      -5.773766     3.295271     0.323489      24.41
 H      -4.686162     4.791060     0.334066      27.38
 H      -4.280896     3.280702     0.984716      25.34
 C      -3.521097     2.513203    -3.036447      21.02
 O      -3.472810     3.596475    -3.821216      69.62
 H      -3.680984     4.594926    -3.317914      17.83
 C      -3.149551     1.219650    -3.582318      23.87
 H      -2.633668     1.182046    -4.591295      26.75
 C      -3.638567    -0.024301    -1.515280      41.19
 C      -3.800473    -1.237129    -0.739354      83.45
 H      -4.563995    -2.070514    -1.391735      19.36
 O      -4.691618    -1.148092     0.489362     141.56
 H      -4.120180    -0.841843     1.285872      23.08
 C      -2.553807    -2.007530    -0.590409      80.63
 H      -2.091830    -2.169549    -1.539368      24.30
 C      -2.879974    -3.446335     0.005108     108.03
 O      -3.854691    -4.126002    -0.851078     129.31
 H      -3.549962    -4.077571    -1.917810      21.53
 H      -3.124688    -3.532392     1.032689      26.09
 H      -1.990936    -4.236742     0.035584      24.50
 C       1.840482    -1.348143    -1.378350      37.97
 H       2.364478    -1.799319    -2.208907      20.12
 C       1.708481     0.441687     0.223493      39.27
 H       2.079621     1.324772     0.598318      22.06
 C       0.396725     0.031623     0.736027     -42.17
 O      -0.255231     0.930979     1.765447     146.17
 C      -0.701064     2.328958     1.369602     102.42
 H      -1.592357     2.589325     2.166176      23.88
 H       0.204020     2.942827     1.201264      24.28
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 H      -1.229222     2.005499     0.622002      28.02
 C      -0.255222    -1.137609    -0.026706     -14.69
 O      -1.537022    -1.372566     0.349548     141.21
 C       0.459099    -1.719392    -1.069402      66.44
 H       0.161046    -2.560384    -1.796925      21.48
 C       2.418974    -0.236725    -0.744969      38.15
 C       3.697691     0.359979    -1.084220      75.51
 H       3.907269     0.252189    -2.319912      21.56
 O       3.853299     1.771833    -0.946832     250.37
 H       4.327327     1.806330    -0.149767      23.33
 C       5.060896    -0.330906    -0.393325      90.13
 H       4.934298    -0.161301     0.579281      27.71
 O       4.929766    -1.692843    -0.547546     372.78
 H       5.063113    -1.945438    -1.514375      27.86
 C       6.317169     0.277176    -0.936422     106.69
 O       6.608763     1.561426    -0.364325     325.31
 H       6.845634     1.481330     0.587054      33.39
 H       6.580460     0.338810    -2.155966      26.01
 H       7.127203    -0.257275    -0.822675      29.24
55
name= lig-ACN-Water-frame_529
 C      -3.312402    -0.005361    -2.937616      65.68
 H      -2.820379    -0.945723    -3.267042      25.27
 C      -3.998218     1.302564    -0.993187      69.00
 H      -4.736047     1.299121    -0.000589      19.76
 C      -4.036357     2.494426    -1.684259      15.57
 O      -4.422180     3.716265    -1.190368     189.17
 C      -4.876260     3.791905     0.362685     109.09
 H      -5.943452     3.627730     0.383897      26.17
 H      -4.932982     4.718986     0.631492      28.58
 H      -4.116765     3.167168     0.865594      24.46
 C      -3.536319     2.459769    -3.079861       6.82
 O      -3.489281     3.587680    -3.933823     104.16
 H      -3.950887     4.473310    -3.444610      20.73
 C      -3.134440     1.215105    -3.622290      51.37
 H      -2.733380     1.225548    -4.642419      23.61
 C      -3.633934     0.078895    -1.574863      27.67
 C      -3.937239    -1.231258    -0.659451      84.90
 H      -4.492404    -2.137243    -1.397961      20.92
 O      -4.634538    -1.139112     0.478208     201.50
 H      -4.178822    -0.609032     1.239088      21.79
 C      -2.519942    -2.084774    -0.494365      76.45
 H      -2.150601    -2.091532    -1.534233      23.56
 C      -2.887502    -3.515461     0.062810     113.21
 O      -3.883113    -4.121155    -0.812854     152.68
 H      -3.434757    -4.197741    -1.710396      27.61
 H      -3.442661    -3.279026     0.970032      24.73
 H      -1.852010    -4.018292    -0.017938      23.49
 C       1.773951    -1.288822    -1.350864      36.22
 H       2.400500    -1.919380    -1.936543      20.15
 C       1.607658     0.538538     0.316085      52.19
 H       2.110359     1.454233     0.736024      17.46
 C       0.355803     0.140690     0.631012       1.53
 O      -0.252280     0.835246     1.654247     240.61
 C      -0.713825     2.148808     1.363794     122.79
 H      -0.930252     2.611257     2.433020      23.88
 H       0.188235     2.901778     1.087946      22.29
 H      -1.301362     2.495392     0.680666      28.49
 C      -0.201767    -1.106053     0.151608     -18.39
 O      -1.597222    -1.418649     0.334561     134.28
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 C       0.489554    -1.687131    -1.068235      51.15
 H      -0.096379    -2.678078    -1.484217      18.01
 C       2.375971    -0.191843    -0.704925       9.52
 C       3.861402     0.283732    -1.142559      71.41
 H       3.917776    -0.020277    -2.381588      20.04
 O       3.799530     1.737564    -0.949071     224.86
 H       4.256832     2.150527    -0.209620      20.69
 C       4.960955    -0.289065    -0.412602     103.38
 H       4.948711     0.006832     0.544968      25.79
 O       4.985266    -1.769671    -0.462193     349.11
 H       5.263180    -2.030858    -1.371776      28.36
 C       6.449771     0.238813    -0.904131      66.74
 O       6.655413     1.596664    -0.381615     341.53
 H       6.858701     1.555676     0.599481      32.19
 H       6.091805     0.490221    -2.061187      27.22
 H       7.050478    -0.472699    -0.653603      32.48
55
name= lig-ACN-Water-frame_530
 C      -3.275009     0.065677    -2.938800      51.04
 H      -3.074624    -0.927178    -3.463637      26.05
 C      -4.099408     1.322285    -0.918261      45.67
 H      -4.421096     1.248151     0.293244      20.45
 C      -3.995714     2.525262    -1.754820       2.37
 O      -4.446016     3.813729    -1.184754     146.20
 C      -4.913246     3.755648     0.307901     115.26
 H      -5.812882     3.265930     0.496418      27.69
 H      -4.700006     4.702968     0.444257      29.55
 H      -4.241080     3.144177     0.995659      26.55
 C      -3.583516     2.455818    -3.113797      11.15
 O      -3.510413     3.482069    -4.024727      79.98
 H      -3.680247     4.441481    -3.503597      21.61
 C      -3.165655     1.238448    -3.703761      57.37
 H      -2.945202     1.298165    -4.740143      24.46
 C      -3.763604     0.088431    -1.542433      -0.70
 C      -3.813665    -1.287555    -0.794818      55.44
 H      -4.802619    -1.673951    -1.457203      19.89
 O      -4.629604    -1.070722     0.580514      91.86
 H      -4.044190    -0.587306     1.192463      26.75
 C      -2.548862    -2.131510    -0.499521      93.21
 H      -2.005926    -2.403327    -1.459003      25.01
 C      -2.864655    -3.481958     0.072771     121.65
 O      -3.826649    -4.152166    -0.751409     200.42
 H      -3.620217    -4.249210    -1.605181      31.89
 H      -3.294856    -3.468794     1.136744      25.43
 H      -2.036941    -4.188075     0.390218      26.52
 C       1.757898    -1.257389    -1.305193      55.91
 H       2.203057    -1.765761    -2.145329      21.84
 C       1.665396     0.578905     0.259129      33.96
 H       1.949950     1.451716     1.026087      20.02
 C       0.302597     0.128376     0.554246     -21.28
 O      -0.387368     0.700056     1.591447     223.95
 C      -0.659106     2.144312     1.420809     112.46
 H      -0.854082     2.510222     2.447521      26.79
 H       0.304379     2.571403     0.769515      22.30
 H      -1.511044     2.048647     0.958848      30.12
 C      -0.266776    -1.019107     0.002809      18.67
 O      -1.603088    -1.385324     0.481343     127.76
 C       0.464895    -1.701238    -0.844783      63.06
 H      -0.038623    -2.646909    -1.483468      22.59
 C       2.399119    -0.130551    -0.674474      25.31
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 C       3.744090     0.283651    -1.152651      98.06
 H       3.938130     0.021537    -2.369009      21.06
 O       3.778264     1.762754    -1.042440     239.45
 H       4.222360     1.746727    -0.082661      20.65
 C       5.077171    -0.355061    -0.315230      91.19
 H       4.839899    -0.152625     0.684467      27.19
 O       5.029958    -1.821911    -0.318929     323.27
 H       5.143554    -1.975818    -1.277294      28.54
 C       6.389248     0.257229    -0.832884     121.78
 O       6.727992     1.599018    -0.402473     262.87
 H       7.068537     1.616192     0.534883      30.38
 H       6.758784     0.212683    -2.023912      27.25
 H       7.140350    -0.311601    -0.595933      31.44
55
name= lig-ACN-Water-frame_531
 C      -3.287334     0.085474    -2.855061      52.65
 H      -3.192152    -0.942361    -3.363053      21.64
 C      -4.125192     1.351667    -1.013145      75.75
 H      -4.289612     1.499480     0.171212      20.20
 C      -4.051354     2.572424    -1.680524      11.35
 O      -4.452775     3.761317    -1.147527     224.62
 C      -4.854547     3.758664     0.145243     146.67
 H      -5.806490     3.349238     0.138259      27.35
 H      -5.212150     4.647033     0.533441      27.67
 H      -4.022223     3.319973     0.761145      24.83
 C      -3.617922     2.479471    -3.131743       5.05
 O      -3.547765     3.491006    -4.065632     139.88
 H      -3.678096     4.456195    -3.625751      18.87
 C      -3.277860     1.222109    -3.702899      70.26
 H      -2.933285     1.117395    -4.692923      31.35
 C      -3.750238     0.087938    -1.569820      47.78
 C      -3.852058    -1.215269    -0.740544      86.36
 H      -4.268988    -2.269868    -1.215700      26.12
 O      -4.541881    -1.022637     0.533804     170.32
 H      -3.979931    -0.878397     1.300908      25.65
 C      -2.508797    -2.086831    -0.519212      45.83
 H      -1.824400    -2.120891    -1.443239      24.79
 C      -2.860169    -3.496941     0.182206     106.66
 O      -3.762261    -4.236058    -0.707290     181.46
 H      -3.262786    -4.069579    -1.550839      30.28
 H      -3.410423    -3.207556     1.159471      25.32
 H      -1.828426    -3.966145     0.092048      25.75
 C       1.738114    -1.259817    -1.248395      52.08
 H       2.191357    -1.643901    -2.165740      24.02
 C       1.598052     0.536384     0.260414      56.31
 H       2.269419     1.417110     0.762469      20.76
 C       0.309917     0.116866     0.569490       3.54
 O      -0.538771     0.635592     1.623777     186.18
 C      -0.665819     2.091553     1.488006     110.86
 H      -0.520736     2.701306     2.334797      28.39
 H      -0.043163     2.696643     0.586892      25.50
 H      -1.602752     2.381165     1.008799      27.77
 C      -0.468715    -0.924787    -0.065109     -28.70
 O      -1.608658    -1.357778     0.551520     114.27
 C       0.523905    -1.822061    -0.857715      34.00
 H       0.217238    -2.822301    -1.502895      23.22
 C       2.350300    -0.164544    -0.706862      34.72
 C       3.727924     0.318757    -1.092853      79.81
 H       3.856903    -0.019358    -2.284300      22.44
 O       3.847983     1.737469    -1.102812     228.79
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 H       4.102699     2.277443    -0.263669      21.61
 C       5.047951    -0.387955    -0.240859      78.17
 H       5.026753     0.000552     0.785606      25.69
 O       5.075622    -1.807660    -0.241082     285.08
 H       5.273645    -2.194190    -1.151783      28.61
 C       6.489734     0.200732    -0.719331      91.21
 O       6.766685     1.612273    -0.414991     247.45
 H       6.839749     1.626219     0.572860      30.83
 H       6.342431     0.138350    -1.914237      28.18
 H       7.103674    -0.412078    -0.279471      32.00
55
name= lig-ACN-Water-frame_532
 C      -3.355938    -0.004725    -2.916984      67.06
 H      -2.805705    -0.950070    -3.289829      27.03
 C      -4.095478     1.357461    -1.020912      78.90
 H      -4.637304     1.222970    -0.031841      21.10
 C      -4.073352     2.522655    -1.829783      25.19
 O      -4.381605     3.790088    -1.285022     170.59
 C      -4.933844     3.753805     0.159189     125.22
 H      -5.554009     2.963895     0.384048      26.66
 H      -5.110320     4.810727     0.200096      26.11
 H      -4.170358     3.492197     0.930144      26.89
 C      -3.678452     2.501207    -3.125560      24.61
 O      -3.599876     3.602503    -4.051165     159.92
 H      -3.908673     4.429716    -3.623708      24.87
 C      -3.371208     1.203868    -3.602405      31.39
 H      -3.052662     1.259785    -4.635363      24.09
 C      -3.719832     0.107243    -1.491664     -31.11
 C      -3.791758    -1.244592    -0.656772      93.39
 H      -4.637524    -1.623703    -1.403157      20.52
 O      -4.492280    -1.000287     0.486498     218.41
 H      -3.867003    -0.646041     1.196857      24.21
 C      -2.509225    -1.961833    -0.373898     112.97
 H      -2.147342    -2.127050    -1.446626      25.71
 C      -2.788406    -3.394489     0.130061      99.58
 O      -3.649807    -4.301460    -0.661930     165.35
 H      -3.392745    -4.513150    -1.717915      24.72
 H      -3.339298    -3.421363     1.189316      24.03
 H      -1.868551    -3.979634     0.526967      25.29
 C       1.734156    -1.380029    -1.316645      39.32
 H       2.408186    -2.091698    -1.842295      17.02
 C       1.516739     0.503248     0.329830      34.05
 H       1.847379     1.488762     0.917892      22.16
 C       0.139690     0.086440     0.655430       1.34
 O      -0.599818     0.697087     1.632891     206.96
 C      -0.741116     2.149595     1.528642      98.58
 H      -0.232968     2.371157     2.379966      26.82
 H       0.121152     2.309297     0.635729      23.62
 H      -1.748612     2.457583     1.555027      26.80
 C      -0.288883    -1.037436    -0.066170       5.77
 O      -1.644587    -1.361870     0.468936     205.95
 C       0.421983    -1.796493    -0.920069      68.57
 H      -0.031057    -2.795855    -1.249782      24.32
 C       2.293953    -0.154971    -0.667884      -1.96
 C       3.858267     0.257790    -1.007394      76.93
 H       4.065809    -0.136222    -2.125050      22.07
 O       3.921254     1.767475    -1.141123     248.85
 H       4.350748     1.911482    -0.328153      26.32
 C       5.000093    -0.266760    -0.183732     105.22
 H       4.713085    -0.158959     0.917230      25.15
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 O       5.076883    -1.776372    -0.191894     276.19
 H       5.486087    -1.878439    -1.131357      26.64
 C       6.475826     0.137994    -0.619975     105.65
 O       6.763933     1.559629    -0.388506     260.17
 H       6.736985     1.901273     0.533137      29.84
 H       6.721149     0.070332    -1.773291      27.78
 H       7.208321    -0.482760    -0.324520      30.92
55
name= lig-ACN-Water-frame_533
 C      -3.365269     0.002649    -2.879659      63.91
 H      -2.966172    -0.911538    -3.433488      25.29
 C      -4.115987     1.325435    -0.996416      63.77
 H      -4.536647     1.485020    -0.055335      23.80
 C      -4.115860     2.531117    -1.810374      -0.10
 O      -4.363620     3.793253    -1.323637     176.69
 C      -4.932363     3.782084     0.111334     116.94
 H      -5.751140     3.183665     0.229978      27.54
 H      -5.619405     4.709960     0.247624      26.65
 H      -4.014792     3.807144     0.676202      26.06
 C      -3.733857     2.504448    -3.248575       7.19
 O      -3.674800     3.657103    -3.960285     140.06
 H      -3.835934     4.441734    -3.460422      26.18
 C      -3.383472     1.205145    -3.708537      40.31
 H      -3.080481     1.065632    -4.774758      21.83
 C      -3.612309     0.075541    -1.544703      46.41
 C      -3.818337    -1.139379    -0.714096      84.19
 H      -4.338438    -2.102210    -1.197977      24.07
 O      -4.561991    -0.960939     0.616362     142.47
 H      -3.975010    -0.438101     1.319517      22.80
 C      -2.568423    -2.072362    -0.513684      64.88
 H      -1.960625    -2.170167    -1.450003      24.67
 C      -2.780656    -3.428540     0.150866     107.02
 O      -3.538837    -4.343906    -0.612672     203.01
 H      -3.023512    -4.304674    -1.566120      25.96
 H      -3.470450    -3.143241     1.054575      24.02
 H      -1.668476    -3.771334     0.329605      23.97
 C       1.776187    -1.416788    -1.241545      37.57
 H       2.419574    -2.103405    -1.865258      23.70
 C       1.442057     0.481430     0.359398      57.75
 H       1.896973     1.351083     0.898293      22.83
 C       0.177420     0.076712     0.683404       5.54
 O      -0.694549     0.707671     1.612153     191.05
 C      -0.666040     2.211023     1.653296     120.02
 H      -0.299670     2.777974     2.399158      28.12
 H      -0.755094     2.872721     0.643466      25.45
 H      -1.742261     2.378757     1.688806      26.23
 C      -0.321705    -1.134670     0.115869      -4.03
 O      -1.574885    -1.313881     0.392039      81.63
 C       0.390959    -1.782452    -1.023047      70.96
 H      -0.043771    -2.649002    -1.470413      21.65
 C       2.316094    -0.254118    -0.629923      12.68
 C       3.794636     0.227016    -1.022848      74.67
 H       4.025826    -0.183724    -2.082422      24.81
 O       3.984423     1.710444    -1.087862     210.69
 H       4.588806     2.166994    -0.471257      24.35
 C       5.028398    -0.296350    -0.053712      81.72
 H       4.924741     0.175347     1.041849      23.74
 O       5.035027    -1.683986    -0.212655     307.02
 H       5.386210    -1.974243    -1.070104      30.10
 C       6.426156     0.165164    -0.502244     110.94
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 O       6.759461     1.523675    -0.354276     237.74
 H       7.053085     1.526117     0.597025      29.47
 H       6.479855    -0.150355    -1.573901      32.02
 H       6.961415    -0.379922     0.177826      31.81
55
name= lig-ACN-Water-frame_534
 C      -3.297960     0.121751    -2.996079      55.43
 H      -3.340415    -0.932250    -3.354192      22.99
 C      -4.093000     1.368366    -1.042428      75.89
 H      -4.108416     1.306963    -0.066440      26.34
 C      -4.106043     2.485232    -1.821900      24.38
 O      -4.430696     3.780014    -1.285557     242.99
 C      -4.947318     3.884775    -0.039342     124.35
 H      -5.401538     2.977125     0.209177      25.73
 H      -5.378633     4.994959     0.088605      25.73
 H      -4.270979     3.745560     0.833096      27.04
 C      -3.788417     2.435615    -3.187683      13.42
 O      -3.748868     3.681050    -3.908818     169.38
 H      -3.901244     4.459851    -3.314693      21.71
 C      -3.379166     1.196635    -3.857175      45.24
 H      -3.094093     1.122227    -4.966309      23.68
 C      -3.687386     0.146590    -1.530270       2.07
 C      -3.873483    -1.241464    -0.612052      84.13
 H      -4.800364    -1.659907    -1.230330      22.98
 O      -4.598394    -0.932647     0.627062     184.12
 H      -3.913790    -0.706872     1.373826      23.69
 C      -2.512479    -2.065073    -0.625449      96.27
 H      -2.223202    -2.206798    -1.680310      23.64
 C      -2.755809    -3.414458     0.209530      97.99
 O      -3.443751    -4.402609    -0.617668     266.03
 H      -3.111029    -4.409174    -1.472010      31.96
 H      -3.183683    -3.310026     1.308840      23.19
 H      -1.728466    -3.899025     0.515105      23.62
 C       1.768637    -1.408262    -1.134593      52.97
 H       2.207654    -1.664963    -2.128672      21.88
 C       1.600646     0.474404     0.316867      65.10
 H       2.021407     1.377611     0.631915      23.91
 C       0.263708     0.037611     0.738238     -27.86
 O      -0.685332     0.783441     1.547467     158.68
 C      -0.800723     2.269625     1.759711     106.16
 H       0.136942     2.432645     2.212889      25.25
 H      -0.492160     2.611500     0.650125      24.73
 H      -1.657956     2.404131     2.332724      26.54
 C      -0.298939    -1.153969     0.064982     -17.85
 O      -1.710624    -1.346053     0.364149     135.30
 C       0.453792    -1.760988    -0.961422      71.33
 H       0.063111    -2.359369    -1.664381      24.56
 C       2.366842    -0.282205    -0.521063      24.86
 C       3.769961     0.250927    -0.898152      94.65
 H       3.891140    -0.159012    -1.942721      24.73
 O       3.956228     1.652154    -1.067884     233.51
 H       4.659917     1.783205    -0.271381      18.36
 C       4.914363    -0.268332    -0.066926      99.81
 H       4.640016    -0.288286     1.134789      22.81
 O       4.976592    -1.719209    -0.177132     337.83
 H       5.240765    -1.789588    -1.105263      29.43
 C       6.391789     0.109068    -0.369604     110.39
 O       6.785897     1.553407    -0.289890     251.70
 H       7.144966     1.869310     0.585698      29.65
 H       6.718512    -0.170674    -1.366266      30.50
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 H       7.104701    -0.512490     0.132496      29.78
55
name= lig-ACN-Water-frame_535
 C      -3.357019     0.059568    -3.011533      55.85
 H      -2.976157    -0.812537    -3.546680      22.53
 C      -4.003276     1.356594    -0.940082      49.79
 H      -4.300877     1.538065    -0.008117      20.33
 C      -4.109253     2.525123    -1.819214      -0.59
 O      -4.427071     3.764186    -1.412494     206.33
 C      -4.990378     3.897091     0.022260     113.37
 H      -5.946348     3.466448     0.149487      24.74
 H      -5.544782     4.983034    -0.145317      25.61
 H      -4.067627     4.059501     0.592265      24.45
 C      -3.778118     2.493800    -3.232856      20.84
 O      -3.825236     3.609387    -3.887841     138.20
 H      -4.031998     4.475747    -3.306611      18.99
 C      -3.415920     1.310606    -3.824080      42.01
 H      -3.179067     1.401539    -4.947390      25.14
 C      -3.743854     0.090906    -1.621434      18.23
 C      -3.973091    -1.182355    -0.701111      83.47
 H      -4.705098    -1.951448    -1.281141      25.36
 O      -4.546399    -0.933569     0.585384     193.63
 H      -3.882212    -0.894306     1.322059      23.74
 C      -2.661801    -2.089161    -0.477722      91.51
 H      -2.150560    -2.123670    -1.432095      26.59
 C      -2.642191    -3.466601     0.124025     118.12
 O      -3.413637    -4.472691    -0.578665     248.46
 H      -3.120965    -4.411616    -1.473129      32.07
 H      -3.490928    -3.183457     0.888077      24.13
 H      -1.619865    -3.749089     0.505343      26.48
 C       1.852030    -1.325689    -1.188626      36.75
 H       2.371480    -1.844243    -2.030695      19.26
 C       1.618011     0.521934     0.463409      65.60
 H       1.849636     1.450635     0.779782      23.18
 C       0.290548     0.078680     0.732378      19.60
 O      -0.674011     0.757745     1.472282     177.06
 C      -0.676223     2.197350     1.790016     123.00
 H       0.149493     2.690715     2.335288      25.58
 H      -1.144421     2.945678     0.938899      25.25
 H      -1.474679     2.446393     2.427674      27.78
 C      -0.352358    -1.016715     0.064177      -3.50
 O      -1.694939    -1.323264     0.289184     186.14
 C       0.438933    -1.776998    -0.850021      52.80
 H      -0.044112    -2.433832    -1.498263      24.03
 C       2.433821    -0.276153    -0.428383      15.33
 C       3.797807     0.189686    -0.918520      93.09
 H       4.031353    -0.225951    -1.891060      22.35
 O       3.876150     1.666492    -1.005512     266.00
 H       4.373105     2.204962    -0.339276      20.64
 C       4.879498    -0.391666     0.029987      76.46
 H       4.524987     0.046681     1.152972      20.40
 O       4.902278    -1.827861    -0.182003     296.76
 H       5.177714    -2.115070    -1.121235      27.44
 C       6.431044     0.144574    -0.279815      96.93
 O       6.805376     1.570032    -0.221725     287.97
 H       6.652125     1.799396     0.713459      31.39
 H       6.539994    -0.109263    -1.274006      31.96
 H       6.973955    -0.475315     0.489048      28.00
55
name= lig-ACN-Water-frame_536
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 C      -3.452141     0.077746    -3.033559      76.08
 H      -2.986958    -0.784517    -3.425479      26.59
 C      -3.966522     1.338678    -1.014558      69.50
 H      -4.411436     1.199366    -0.059680      21.96
 C      -4.054755     2.462211    -1.768203      15.15
 O      -4.497591     3.786343    -1.412574     216.38
 C      -5.044831     4.053449    -0.086593     115.71
 H      -5.670575     3.193102     0.243813      25.86
 H      -5.264110     5.245486    -0.014878      25.93
 H      -4.343086     3.782676     0.796350      26.28
 C      -3.781758     2.486732    -3.123515      14.62
 O      -3.913311     3.659338    -3.999648     163.57
 H      -3.845186     4.571622    -3.382017      18.38
 C      -3.423983     1.257936    -3.700971      49.89
 H      -3.014411     1.185108    -4.742148      22.51
 C      -3.782356     0.049957    -1.633284     -10.11
 C      -3.942485    -1.221368    -0.793103      82.66
 H      -4.636177    -2.026161    -1.331616      24.60
 O      -4.547979    -0.938782     0.502884     176.94
 H      -3.873588    -0.529868     1.080412      25.90
 C      -2.628333    -2.015581    -0.587226      63.67
 H      -2.292922    -2.238168    -1.580810      25.80
 C      -2.752362    -3.489744     0.160817     101.81
 O      -3.377113    -4.547591    -0.587990     221.05
 H      -3.048933    -4.541110    -1.623985      26.81
 H      -2.964511    -3.577670     1.353123      24.02
 H      -1.702420    -3.760555     0.151722      24.93
 C       1.775008    -1.288399    -1.132613      56.23
 H       2.484461    -1.946056    -1.624861      19.51
 C       1.583628     0.492319     0.583767      67.58
 H       2.042657     1.249606     1.133964      23.55
 C       0.229983     0.158339     0.666533      20.58
 O      -0.678053     0.798038     1.475168     200.79
 C      -0.594414     2.180637     1.826521     128.56
 H       0.455935     2.633679     2.056194      24.07
 H      -1.053385     2.711756     0.879617      26.18
 H      -1.181033     2.067007     2.566170      29.12
 C      -0.346794    -0.978947    -0.013063      -0.55
 O      -1.640707    -1.187400     0.331313     128.12
 C       0.529949    -1.734687    -0.838478      76.85
 H       0.176082    -2.752343    -1.149643      25.67
 C       2.392294    -0.215329    -0.459806     -16.34
 C       3.864339     0.196886    -0.889732      88.63
 H       3.985043    -0.078957    -1.875748      24.44
 O       3.766309     1.710569    -0.979521     259.16
 H       4.172167     1.873358    -0.172227      23.78
 C       4.985653    -0.433470     0.054430      84.15
 H       4.750801    -0.531298     1.285858      22.07
 O       4.838986    -1.926380    -0.138062     279.28
 H       5.234305    -1.960540    -1.072682      27.16
 C       6.381596     0.132477    -0.213818     120.49
 O       6.753279     1.534657    -0.148858     285.91
 H       6.837138     1.866473     0.792550      28.19
 H       6.764550    -0.184358    -1.095981      30.65
 H       7.201978    -0.371771     0.468626      26.61
55
name= lig-ACN-Water-frame_537
 C      -3.485909    -0.016604    -2.955044      63.02
 H      -3.489975    -0.903323    -3.531084      26.49
 C      -4.072646     1.249140    -1.014558      57.05
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 H      -4.201102     1.348809     0.120563      24.05
 C      -4.059361     2.606087    -1.741816      -6.03
 O      -4.556357     3.800110    -1.356468     198.99
 C      -5.032912     4.068063    -0.099482     119.46
 H      -6.153772     3.748256    -0.082454      23.26
 H      -5.439248     5.211164    -0.119703      25.22
 H      -4.133214     4.012446     0.619630      24.36
 C      -3.768739     2.546396    -3.187440       1.75
 O      -3.963254     3.613683    -4.035783     166.12
 H      -3.960783     4.547675    -3.536803      21.56
 C      -3.378576     1.254076    -3.727083      36.73
 H      -3.037093     1.301700    -4.759277      23.10
 C      -3.782761     0.035467    -1.641089      57.07
 C      -3.866100    -1.251602    -0.800785      92.97
 H      -4.641162    -1.820910    -1.400005      25.57
 O      -4.583767    -0.965949     0.383143     159.41
 H      -4.042909    -0.611139     1.156302      23.09
 C      -2.519559    -2.021313    -0.604701      82.48
 H      -1.887042    -2.110526    -1.459974      25.69
 C      -2.661963    -3.461590     0.121827      96.89
 O      -3.423442    -4.581311    -0.598099     191.61
 H      -2.873953    -4.493951    -1.567196      25.10
 H      -3.083812    -3.389602     1.229619      24.18
 H      -1.653129    -3.749848     0.111536      24.71
 C       1.865701    -1.295614    -1.034461      29.95
 H       2.416807    -1.827970    -1.792446      23.02
 C       1.642828     0.418794     0.549455      42.38
 H       2.087920     1.063241     1.343031      23.00
 C       0.207588     0.218881     0.588692     -17.02
 O      -0.679516     0.788521     1.526359     173.89
 C      -0.534975     2.218431     1.854263     109.90
 H       0.619700     2.332511     1.881412      23.77
 H      -0.916534     2.931542     1.009139      26.64
 H      -0.824795     2.671455     2.611507      30.19
 C      -0.316081    -0.923488    -0.084029      -6.69
 O      -1.717313    -1.147012     0.270480     118.37
 C       0.466819    -1.765303    -0.833262      45.75
 H       0.203011    -2.886779    -1.233605      19.39
 C       2.348711    -0.116378    -0.456830      43.15
 C       3.770118     0.257906    -0.771537      92.24
 H       4.027633    -0.122979    -1.655560      27.27
 O       3.757248     1.698541    -0.894448     230.97
 H       4.054303     2.300822    -0.133631      23.94
 C       4.970449    -0.471175     0.064184      58.90
 H       4.677258    -0.117299     1.244418      22.13
 O       4.871730    -1.930384    -0.151818     313.92
 H       5.128573    -2.224075    -1.020939      31.65
 C       6.521057     0.007425    -0.185305      87.75
 O       6.640870     1.520641    -0.089275     260.08
 H       6.973594     1.706601     0.851819      28.22
 H       6.683459    -0.228715    -1.147270      32.44
 H       7.108970    -0.670538     0.634325      27.76
55
name= lig-ACN-Water-frame_538
 C      -3.491110     0.041017    -3.076971      38.28
 H      -3.487723    -0.928762    -3.574796      26.08
 C      -4.147825     1.447978    -1.004261      52.38
 H      -4.348393     1.543745     0.181545      24.42
 C      -4.108021     2.498090    -1.813431      27.21
 O      -4.548995     3.831441    -1.416080     143.48
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 C      -5.136041     4.170740    -0.020970     103.95
 H      -6.076566     3.539764     0.382272      24.15
 H      -5.011478     5.301127    -0.162474      25.09
 H      -4.506379     3.800997     0.950149      24.56
 C      -3.738260     2.474232    -3.173779      22.70
 O      -3.982590     3.557202    -4.053999     187.84
 H      -4.080702     4.384008    -3.598513      26.11
 C      -3.370805     1.265926    -3.741806      64.78
 H      -3.253958     1.148033    -4.773075      23.50
 C      -3.757810     0.067298    -1.601799     -25.10
 C      -3.861092    -1.277599    -0.866464      84.93
 H      -4.254319    -2.126117    -1.407863      25.92
 O      -4.644803    -1.051206     0.352205     190.83
 H      -3.964191    -0.747190     1.060609      26.22
 C      -2.433065    -2.064801    -0.606251      93.01
 H      -2.161297    -2.122136    -1.652025      25.55
 C      -2.537033    -3.466017     0.027707     116.47
 O      -3.409347    -4.459283    -0.577853     255.31
 H      -3.192597    -4.699304    -1.521556      28.73
 H      -3.286383    -3.175420     0.836389      24.50
 H      -1.707850    -3.854471     0.546147      26.81
 C       1.845094    -1.377198    -1.075962      51.85
 H       2.447584    -1.772437    -1.872075      20.55
 C       1.541524     0.492710     0.589108      47.42
 H       2.065918     1.350564     1.211485      17.62
 C       0.194831     0.226404     0.636803       2.27
 O      -0.681722     0.815447     1.600879     189.21
 C      -0.348188     2.284318     1.812413     114.70
 H       0.769404     2.602358     1.823335      23.57
 H      -0.860296     2.810419     0.963481      27.92
 H      -0.767385     2.310092     2.642089      29.09
 C      -0.428372    -0.884522    -0.081997      -7.11
 O      -1.713827    -1.134980     0.183873     181.21
 C       0.516700    -1.741300    -0.815595      61.58
 H      -0.089351    -2.548012    -1.575364      23.39
 C       2.396945    -0.248743    -0.420440       5.22
 C       3.800024     0.290681    -0.745257      99.91
 H       3.871314     0.108889    -1.710640      23.97
 O       3.811823     1.759404    -0.802896     228.28
 H       4.344419     1.958324     0.115187      18.12
 C       4.941584    -0.450524     0.085474      83.51
 H       4.813893    -0.436827     1.325304      21.46
 O       4.909661    -1.877432    -0.132067     321.96
 H       5.136532    -1.851906    -1.088451      27.15
 C       6.478222    -0.038219    -0.218946      91.22
 O       6.571770     1.393833    -0.029853     342.63
 H       6.819043     1.701087     0.888587      30.37
 H       6.895460    -0.351575    -1.134519      29.72
 H       7.293302    -0.546103     0.557552      26.01
55
name= lig-ACN-Water-frame_539
 C      -3.499615     0.117448    -2.967009      72.79
 H      -3.086135    -0.812235    -3.426558      24.60
 C      -4.095795     1.331375    -1.029300      50.70
 H      -4.681790     1.358913     0.033041      19.72
 C      -4.227894     2.582226    -1.838594      -5.81
 O      -4.564036     3.855490    -1.402210     162.45
 C      -5.118408     4.176541    -0.008473      96.59
 H      -6.311009     3.866413    -0.168935      22.48
 H      -5.313700     5.233206     0.229164      26.16
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 H      -4.274623     3.697403     0.689289      22.64
 C      -3.765168     2.465259    -3.225963       2.44
 O      -3.972110     3.498551    -4.052223     199.59
 H      -3.864532     4.337085    -3.605448      22.81
 C      -3.411184     1.213246    -3.847476      59.93
 H      -3.114084     1.265489    -4.863304      25.79
 C      -3.784422     0.193041    -1.655703      42.21
 C      -3.871768    -1.354297    -0.885616      86.03
 H      -4.592700    -1.715177    -1.495747      26.92
 O      -4.633962    -1.184585     0.335348     176.34
 H      -4.170470    -0.738896     1.048381      26.96
 C      -2.476145    -2.026705    -0.777093      89.59
 H      -1.848983    -2.114785    -1.680586      24.32
 C      -2.583920    -3.416880     0.118396     106.66
 O      -3.393852    -4.340166    -0.588383     297.75
 H      -3.006229    -4.317333    -1.398741      34.14
 H      -2.997976    -3.182742     1.084343      25.66
 H      -1.543073    -3.838801     0.159284      24.93
 C       1.799710    -1.348334    -1.099925      51.07
 H       2.303918    -2.060198    -1.738604      19.27
 C       1.530963     0.477397     0.465927      53.55
 H       1.981364     1.522379     0.827788      19.33
 C       0.156437     0.154317     0.772576      39.65
 O      -0.564567     0.918099     1.600392     237.88
 C      -0.294942     2.267150     1.816858     127.59
 H       0.824603     2.419452     1.873631      24.26
 H      -0.726509     2.946137     1.065070      28.36
 H      -0.580288     2.640515     2.649765      30.24
 C      -0.294468    -0.886129    -0.037558      22.40
 O      -1.696778    -1.129558     0.145059     168.89
 C       0.446687    -1.632088    -0.885219      65.87
 H      -0.014891    -2.541512    -1.608859      20.93
 C       2.380324    -0.312653    -0.261687      18.86
 C       3.848173     0.267331    -0.789596      76.79
 H       4.118082    -0.036541    -1.682141      25.56
 O       3.898753     1.799941    -0.650323     238.10
 H       4.364273     2.196274     0.156329      22.36
 C       5.009448    -0.456847     0.095178      87.52
 H       4.678232    -0.178255     1.244186      23.20
 O       4.918181    -1.842022    -0.175771     307.36
 H       5.133354    -2.151540    -1.125216      27.17
 C       6.377313    -0.030869    -0.185265      89.58
 O       6.556177     1.339916    -0.007963     335.84
 H       6.993074     1.499145     0.843116      31.70
 H       6.545820    -0.236621    -1.247223      30.93
 H       7.033051    -0.775389     0.560767      27.29
55
name= lig-ACN-Water-frame_540
 C      -3.353061     0.074703    -3.018248      28.66
 H      -2.995019    -0.949319    -3.354568      20.37
 C      -4.198553     1.408151    -1.044229      63.67
 H      -4.503530     1.292814     0.077991      21.18
 C      -4.245535     2.553844    -1.805152       8.06
 O      -4.577623     3.939833    -1.395682     185.70
 C      -5.100396     4.080662    -0.125361     121.35
 H      -6.259928     3.614319     0.089819      23.89
 H      -4.888913     5.116938    -0.074278      26.42
 H      -4.652984     3.483071     0.879182      22.38
 C      -3.901757     2.451999    -3.221991       3.23
 O      -3.936774     3.570916    -4.113080     206.47
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 H      -3.723683     4.517584    -3.672595      18.08
 C      -3.484552     1.256440    -3.822252      64.83
 H      -2.938301     1.178780    -4.764620      28.40
 C      -3.802911     0.068415    -1.609870      13.19
 C      -3.948116    -1.194845    -0.979048     109.13
 H      -4.348723    -1.933901    -1.521120      28.13
 O      -4.564118    -1.329526     0.342142     175.29
 H      -3.943043    -0.960228     0.979709      26.49
 C      -2.546614    -1.985960    -0.714531      77.50
 H      -2.160772    -2.220024    -1.741965      23.55
 C      -2.540457    -3.275803     0.105065     109.58
 O      -3.431495    -4.259410    -0.591688     269.52
 H      -3.211621    -4.362237    -1.540263      29.98
 H      -2.769881    -3.139227     1.101312      27.32
 H      -1.466362    -3.593694     0.106566      24.59
 C       1.832128    -1.334513    -1.034912      50.36
 H       2.521453    -1.801320    -1.759003      20.27
 C       1.600880     0.504788     0.402316      63.59
 H       1.970946     1.531849     0.780135      19.80
 C       0.338395     0.127816     0.794311       5.74
 O      -0.584366     0.931596     1.643225     180.30
 C      -0.199882     2.382893     1.855275     122.81
 H       0.901986     2.390760     1.926657      24.51
 H      -0.380852     2.879999     0.956711      28.96
 H      -0.687101     2.633362     2.678271      28.40
 C      -0.391975    -0.944049     0.059777      -6.91
 O      -1.706498    -1.101702     0.116602     140.94
 C       0.411022    -1.563587    -1.017235      64.03
 H      -0.054659    -2.562523    -1.484264      19.06
 C       2.470675    -0.293104    -0.405545      35.06
 C       3.851995     0.288532    -0.656896     104.81
 H       3.860363     0.228166    -1.635762      22.67
 O       3.933407     1.736459    -0.582597     296.64
 H       4.106061     1.929472     0.335346      24.78
 C       4.892421    -0.454037     0.072706      97.29
 H       4.736533    -0.400298     1.252479      23.46
 O       4.887894    -1.911985    -0.188120     293.77
 H       5.001493    -1.874720    -1.211274      26.12
 C       6.365036    -0.065058    -0.222936      88.39
 O       6.616137     1.404043     0.046141     308.57
 H       7.128973     1.668264     0.851393      31.50
 H       6.621023    -0.277727    -1.288274      30.07
 H       7.191160    -0.772881     0.326315      27.37
55
name= lig-ACN-Water-frame_541
 C      -3.298657     0.079860    -2.990529      73.64
 H      -2.999658    -0.776406    -3.620930      22.92
 C      -4.297433     1.342706    -1.056396      72.00
 H      -4.451029     1.553295    -0.020159      21.32
 C      -4.256168     2.593772    -1.882664       4.27
 O      -4.533187     3.835373    -1.475835     190.27
 C      -5.117461     4.032988    -0.084896      91.07
 H      -6.364655     3.857999    -0.175406      23.97
 H      -5.107479     4.993179     0.322996      27.05
 H      -4.326747     3.354372     0.554868      23.17
 C      -4.008029     2.519487    -3.262183       4.88
 O      -3.903902     3.638193    -4.134189     170.34
 H      -3.853057     4.537821    -3.492743      21.39
 C      -3.458937     1.238351    -3.688335      23.97
 H      -3.266665     1.406503    -4.787586      19.96
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 C      -3.839564     0.186057    -1.691657      21.66
 C      -3.909153    -1.327991    -0.894086      98.22
 H      -4.496165    -1.815268    -1.533891      27.50
 O      -4.548346    -1.392353     0.369806     158.85
 H      -3.886076    -1.115322     1.103871      23.49
 C      -2.543835    -1.855390    -0.681521      98.97
 H      -2.012153    -1.922262    -1.679836      23.45
 C      -2.535067    -3.270545    -0.013473     115.04
 O      -3.474640    -4.170293    -0.520860     232.66
 H      -3.097635    -4.414234    -1.522036      25.60
 H      -3.051218    -3.092471     0.878148      25.71
 H      -1.515055    -3.678732     0.052668      24.64
 C       1.860918    -1.354800    -1.109514      50.82
 H       2.274506    -1.988186    -1.932555      18.23
 C       1.668806     0.568854     0.475088      52.92
 H       2.154795     1.417838     0.927550      18.61
 C       0.263532     0.132285     0.760932      -9.18
 O      -0.533660     0.901272     1.647740     161.66
 C      -0.106610     2.377345     1.859934     117.40
 H       0.828091     2.530321     2.305114      25.77
 H      -0.299712     2.979889     1.058671      27.70
 H      -0.747767     2.677206     2.589485      27.77
 C      -0.313053    -0.938516    -0.003662       2.63
 O      -1.769793    -0.990100     0.150064     172.36
 C       0.469898    -1.562978    -0.955927      60.96
 H       0.015795    -2.202015    -1.750159      20.66
 C       2.402574    -0.150227    -0.481465      11.12
 C       3.816302     0.300510    -0.733313      89.62
 H       4.205714     0.016670    -1.589287      24.36
 O       3.921859     1.689473    -0.474597     288.80
 H       4.150291     2.085642     0.337463      23.42
 C       4.960393    -0.562700     0.129166      58.47
 H       4.724123    -0.445366     1.246207      23.40
 O       4.818163    -1.950236    -0.211999     336.85
 H       4.787798    -2.136582    -1.199078      27.60
 C       6.418352     0.049900    -0.237551      88.76
 O       6.685112     1.401314     0.034519     341.99
 H       6.947543     1.467924     1.002216      30.83
 H       6.620102    -0.053607    -1.362727      28.66
 H       7.121338    -0.642663     0.425458      26.36
55
name= lig-ACN-Water-frame_542
 C      -3.390905     0.172882    -2.916430      44.05
 H      -2.966126    -0.779375    -3.232407      24.93
 C      -4.326695     1.368253    -1.166427      66.30
 H      -4.759322     1.245586    -0.263303      24.44
 C      -4.338094     2.540028    -1.929204      13.51
 O      -4.542895     3.859007    -1.440066     199.65
 C      -5.081687     3.969382    -0.103336     112.95
 H      -6.213050     3.487093    -0.145971      24.72
 H      -4.944390     5.006268     0.028158      27.20
 H      -4.680446     3.218520     0.796847      22.83
 C      -3.945745     2.527270    -3.300846      21.14
 O      -3.914707     3.617940    -4.097303     168.10
 H      -3.787993     4.585128    -3.589634      20.46
 C      -3.433673     1.378657    -3.803246      51.39
 H      -3.062749     1.081723    -4.834314      21.66
 C      -3.864593     0.074768    -1.600204       6.19
 C      -3.906703    -1.283252    -0.870494      85.22
 H      -4.363237    -2.015205    -1.400645      26.73
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 O      -4.603685    -1.390439     0.457672     136.77
 H      -4.139595    -0.735691     1.102225      26.71
 C      -2.376263    -1.836865    -0.801511      60.47
 H      -1.880205    -1.733393    -1.808069      23.34
 C      -2.552317    -3.250238     0.016097     107.01
 O      -3.545484    -4.168536    -0.537527     243.11
 H      -3.241212    -4.447010    -1.536116      26.30
 H      -2.620446    -3.025739     1.041215      27.12
 H      -1.535769    -3.749148    -0.014293      24.23
 C       1.846045    -1.214768    -1.208780      57.66
 H       2.540119    -1.715023    -1.922550      17.70
 C       1.589718     0.501750     0.530157      71.45
 H       1.964487     1.236654     1.124621      21.86
 C       0.279437     0.254273     0.712828      21.16
 O      -0.433383     0.924658     1.648714     249.40
 C      -0.144335     2.258464     1.908830     135.46
 H       0.756788     2.297702     2.380943      27.04
 H       0.056354     2.636813     1.039788      30.02
 H      -0.978339     2.692886     2.379248      27.12
 C      -0.342187    -0.782511    -0.016474     -11.33
 O      -1.704091    -0.851575     0.194283     119.65
 C       0.468744    -1.657473    -0.911363      71.81
 H       0.018246    -2.263802    -1.606105      22.84
 C       2.348949    -0.148298    -0.528052      23.89
 C       3.929900     0.216295    -0.724764      92.15
 H       4.033114     0.270556    -1.728739      25.15
 O       3.891073     1.748241    -0.454108     180.29
 H       4.424917     1.777848     0.381183      21.37
 C       4.980857    -0.551541     0.086605      95.69
 H       4.907831    -0.471176     1.188011      25.36
 O       4.771725    -1.974789    -0.164161     318.22
 H       4.828660    -2.088164    -1.143254      28.58
 C       6.429857     0.012934    -0.224495      91.45
 O       6.735413     1.416160     0.027654     314.99
 H       6.831562     1.806393     0.939894      28.86
 H       6.529140    -0.113199    -1.361003      29.01
 H       7.273998    -0.682953     0.156835      28.19
55
name= lig-ACN-Water-frame_543
 C      -3.434146     0.195666    -2.984335      60.86
 H      -2.958346    -0.635796    -3.464657      25.19
 C      -4.457961     1.332528    -1.108399      66.64
 H      -4.923550     1.555744    -0.247799      21.54
 C      -4.377424     2.531912    -1.965241      -3.20
 O      -4.554126     3.812662    -1.399704     199.94
 C      -5.103553     3.904650    -0.103574     116.26
 H      -6.278102     3.740354     0.018361      23.71
 H      -5.114741     4.952847     0.227719      25.96
 H      -4.259786     3.435194     0.675758      22.49
 C      -3.821221     2.528730    -3.296637      -6.77
 O      -3.949382     3.644886    -4.112081     233.92
 H      -3.654696     4.535406    -3.591379      19.79
 C      -3.393554     1.229493    -3.833607      51.32
 H      -2.788482     1.377339    -4.757604      23.09
 C      -3.945603     0.114045    -1.603360      38.45
 C      -3.866898    -1.243302    -0.846630      90.62
 H      -4.389921    -1.918473    -1.459076      26.59
 O      -4.588996    -1.297026     0.477953     194.91
 H      -4.325487    -0.531604     0.979181      28.14
 C      -2.413701    -1.805611    -0.665107      94.71
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 H      -1.957752    -2.025997    -1.660889      23.85
 C      -2.406099    -3.218934    -0.028538     101.39
 O      -3.608258    -4.137455    -0.536799     228.73
 H      -3.338994    -4.296519    -1.423037      31.90
 H      -2.810957    -3.136010     0.971905      25.62
 H      -1.497516    -3.873106    -0.298058      24.10
 C       1.721868    -1.114146    -1.259612      56.15
 H       2.199937    -1.683886    -2.087276      23.00
 C       1.699990     0.490218     0.512147      60.83
 H       2.292039     1.144963     1.072410      20.69
 C       0.320283     0.284778     0.654818      22.38
 O      -0.486717     0.838757     1.705622     214.49
 C      -0.131867     2.265887     1.922296     127.28
 H       0.444160     2.488964     2.740363      27.42
 H       0.094241     2.749638     1.133741      30.65
 H      -1.058297     2.679884     2.293351      27.00
 C      -0.330022    -0.733503    -0.103179      14.73
 O      -1.648935    -0.851710     0.110225     163.52
 C       0.420484    -1.587539    -0.896517      67.10
 H       0.110419    -2.515886    -1.024409      22.35
 C       2.493962    -0.163687    -0.447012      23.41
 C       3.819197     0.331986    -0.694232      97.48
 H       4.098028    -0.054652    -1.661708      24.98
 O       3.909608     1.724912    -0.494698     213.04
 H       4.253048     2.232305     0.395912      19.27
 C       4.974159    -0.496880     0.086087      95.44
 H       4.698477    -0.290632     1.074635      27.18
 O       4.799308    -1.953199    -0.079280     289.29
 H       4.665923    -2.118412    -1.027402      29.11
 C       6.465991    -0.083408    -0.261842      96.73
 O       6.747803     1.415154    -0.032398     250.32
 H       6.936862     1.517145     0.912447      29.68
 H       6.656829    -0.109161    -1.404013      29.38
 H       7.174980    -0.733474     0.269590      30.09
55
name= lig-ACN-Water-frame_544
 C      -3.430835     0.002131    -2.994505      55.80
 H      -3.092621    -0.980854    -3.284886      23.01
 C      -4.587661     1.389502    -1.122226      92.38
 H      -4.773074     1.228375    -0.090395      27.62
 C      -4.331169     2.503430    -1.911267       7.28
 O      -4.603308     3.763745    -1.454877     119.61
 C      -5.104623     3.937534     0.005431     100.05
 H      -5.977005     3.256527     0.080861      25.47
 H      -5.138053     5.069090     0.153528      25.98
 H      -4.393879     3.263221     0.739253      24.11
 C      -3.810834     2.512062    -3.276142      28.78
 O      -3.945644     3.630498    -4.133568     199.55
 H      -3.627452     4.494379    -3.689664      23.52
 C      -3.346577     1.318308    -3.792053      42.88
 H      -2.948882     1.174501    -4.775648      24.36
 C      -3.995127     0.192646    -1.725933     -25.59
 C      -3.899650    -1.210228    -0.781677      91.13
 H      -4.452606    -1.957260    -1.393049      25.58
 O      -4.555831    -1.141805     0.409768     221.67
 H      -3.993543    -0.713535     1.102664      24.23
 C      -2.498101    -1.843664    -0.619375      90.03
 H      -2.128123    -1.779041    -1.665295      24.95
 C      -2.479271    -3.307605    -0.049016     120.49
 O      -3.556922    -4.016840    -0.539912     291.89
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 H      -3.419321    -4.277807    -1.420036      31.92
 H      -2.331685    -3.294594     1.100471      26.08
 H      -1.366946    -3.655722    -0.258901      24.45
 C       1.767245    -1.117917    -1.279752      56.97
 H       2.203664    -1.647300    -2.115710      22.85
 C       1.785794     0.524257     0.585341      50.87
 H       2.177072     1.283123     1.311338      21.05
 C       0.364981     0.280904     0.702431     -11.24
 O      -0.473611     0.791822     1.699209     170.18
 C      -0.246440     2.319023     2.001676     109.67
 H       0.465558     2.337757     2.796432      25.09
 H       0.226898     2.619327     1.240427      30.53
 H      -1.225753     2.740200     2.001456      26.90
 C      -0.301125    -0.683845    -0.114694      16.97
 O      -1.679596    -0.874528     0.068594     155.97
 C       0.416004    -1.499636    -0.913854      72.18
 H       0.112209    -2.390097    -1.401959      22.72
 C       2.385546    -0.232919    -0.454015      36.02
 C       3.885822     0.316996    -0.722397      87.19
 H       4.062793     0.368161    -1.821911      22.60
 O       3.943189     1.801755    -0.597702     214.55
 H       4.093652     1.906676     0.409651      23.12
 C       4.957086    -0.429124     0.136786     103.34
 H       5.011408    -0.227174     1.132963      27.47
 O       4.838592    -1.865309     0.004313     275.32
 H       4.640307    -2.140392    -0.949200      27.44
 C       6.440339    -0.047018    -0.309426     105.81
 O       6.758839     1.278935    -0.098035     285.11
 H       6.899277     1.566012     0.844898      28.27
 H       6.729608    -0.508525    -1.302410      29.26
 H       7.022593    -0.680780     0.317474      29.86
55
name= lig-ACN-Water-frame_545
 C      -3.461143     0.081654    -3.025443      62.63
 H      -3.133290    -0.860343    -3.488966      24.41
 C      -4.486071     1.266339    -1.246301      66.79
 H      -4.979365     1.409971    -0.218979      26.25
 C      -4.317629     2.556871    -1.874154       4.54
 O      -4.698619     3.842963    -1.398552     177.05
 C      -5.057337     3.846974    -0.028383     119.93
 H      -6.034528     3.496442     0.191819      26.21
 H      -5.348534     4.990506     0.087883      26.18
 H      -4.154449     3.735405     0.750353      25.43
 C      -3.854741     2.469569    -3.231263       7.05
 O      -3.910062     3.567003    -4.115888     198.34
 H      -3.605110     4.410801    -3.761836      25.69
 C      -3.304548     1.204134    -3.747219      52.72
 H      -3.138231     1.285711    -4.757769      24.96
 C      -4.015933     0.040863    -1.679953      51.12
 C      -3.976436    -1.137243    -0.883711     100.72
 H      -4.578521    -1.973094    -1.349470      26.31
 O      -4.607652    -0.947573     0.470909     141.66
 H      -3.893610    -1.005527     1.213893      23.64
 C      -2.517270    -1.824479    -0.757454      64.26
 H      -2.104693    -2.102938    -1.742773      24.54
 C      -2.414698    -3.240882    -0.008617     101.07
 O      -3.563546    -4.001488    -0.571208     182.10
 H      -3.163036    -4.211568    -1.544641      27.27
 H      -2.631728    -3.387151     1.148322      25.06
 H      -1.613815    -3.884189    -0.583883      22.75
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 C       1.829756    -1.173598    -1.227773      58.01
 H       2.410318    -1.518058    -2.050975      22.30
 C       1.672725     0.465754     0.635541      61.73
 H       2.342907     1.214120     1.238960      21.91
 C       0.354935     0.249452     0.815356      33.41
 O      -0.446008     0.886542     1.719015     239.44
 C      -0.359333     2.217285     1.978371     135.05
 H      -0.093976     2.469175     3.079021      25.96
 H       0.161053     2.762267     1.381422      30.86
 H      -1.378704     2.701589     2.089990      27.89
 C      -0.340318    -0.698322    -0.056333     -23.52
 O      -1.702549    -0.830761     0.160682      74.64
 C       0.454580    -1.501300    -1.088153      67.09
 H      -0.246978    -1.830413    -1.900923      19.26
 C       2.474002    -0.083059    -0.460626      19.33
 C       3.875958     0.266333    -0.768948      69.26
 H       4.080666    -0.238073    -1.820313      25.70
 O       3.964108     1.854558    -0.637407     118.30
 H       4.248256     2.211166     0.168887      27.42
 C       4.994295    -0.359837     0.114698     108.18
 H       4.714352    -0.079102     1.015952      30.79
 O       4.843444    -1.792680     0.077115     235.62
 H       4.799941    -2.032558    -0.944714      29.66
 C       6.431899    -0.158880    -0.242241     107.17
 O       6.821179     1.260714    -0.211583     279.76
 H       6.798743     1.529158     0.746912      30.70
 H       6.478406    -0.272482    -1.380833      28.45
 H       7.031449    -0.762232     0.318208      31.18
55
name= lig-ACN-Water-frame_546
 C      -3.461252     0.010021    -3.024628      56.01
 H      -3.084283    -0.872696    -3.613918      24.87
 C      -4.387557     1.324829    -1.211411      30.56
 H      -5.030903     1.138063    -0.196218      13.85
 C      -4.324368     2.506691    -1.936629      17.60
 O      -4.767876     3.827713    -1.406621     160.17
 C      -5.075874     3.932190     0.013158     125.66
 H      -5.632752     3.140832     0.360001      27.86
 H      -5.386798     5.037001     0.347709      26.84
 H      -4.080012     3.548900     0.547730      25.71
 C      -3.825389     2.484690    -3.234462      33.89
 O      -3.846542     3.484141    -4.101560     221.48
 H      -3.662665     4.340858    -3.626125      24.15
 C      -3.407619     1.294593    -3.768352      51.69
 H      -2.852683     1.221975    -4.632568      26.97
 C      -3.979900     0.058286    -1.774964       6.12
 C      -4.018981    -1.277014    -0.804781      78.73
 H      -4.779810    -1.998804    -1.312349      26.25
 O      -4.680230    -0.831052     0.450763     100.15
 H      -4.015841    -0.458928     1.200791      22.95
 C      -2.509641    -1.761837    -0.691048      91.08
 H      -2.056461    -1.565637    -1.665973      28.13
 C      -2.442823    -3.172497    -0.112976      99.59
 O      -3.586682    -4.051543    -0.634769     166.81
 H      -3.462602    -4.341334    -1.681797      26.31
 H      -2.593026    -2.825598     1.045431      26.52
 H      -1.276053    -3.511779     0.090433      26.41
 C       1.823423    -1.083879    -1.160870      42.52
 H       2.235009    -1.529888    -2.069167      19.52
 C       1.732460     0.461686     0.609094      48.26
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 H       2.067298     1.317415     1.351229      23.68
 C       0.293876     0.124731     0.813419     -16.04
 O      -0.491849     0.828219     1.770322     165.95
 C      -0.503313     2.340767     2.035393     103.74
 H      -0.169627     2.366500     3.162031      23.86
 H       0.178869     2.774630     1.409532      28.32
 H      -1.462184     2.470134     1.621486      26.62
 C      -0.298396    -0.825584    -0.065286      18.61
 O      -1.734787    -0.841876     0.149729     141.38
 C       0.418388    -1.281962    -1.114913      88.06
 H       0.115915    -2.015122    -2.052283      24.28
 C       2.430290    -0.121099    -0.415947      42.37
 C       3.889846     0.370379    -0.759178      91.10
 H       4.136229     0.253336    -1.912750      29.29
 O       3.974209     1.814776    -0.737433     196.86
 H       4.447469     1.937210     0.095873      28.82
 C       4.925053    -0.340196     0.180464     107.97
 H       4.869413    -0.041053     1.106492      33.18
 O       4.808028    -1.790886     0.127395     243.43
 H       4.803894    -2.106077    -0.804936      32.86
 C       6.474351    -0.133749    -0.271281     103.55
 O       6.891790     1.270574    -0.277929     173.45
 H       7.044347     1.691174     0.585108      27.82
 H       6.601937    -0.604743    -1.324871      30.41
 H       7.068854    -0.787027     0.218792      33.31
55
name= lig-ACN-Water-frame_547
 C      -3.452449     0.024008    -3.132940      58.43
 H      -3.093323    -1.001010    -3.433961      24.85
 C      -4.350589     1.305933    -1.152793      49.44
 H      -4.688815     1.411876     0.047071      19.89
 C      -4.392364     2.542366    -1.866972       4.72
 O      -4.827849     3.759313    -1.487630     175.85
 C      -4.997528     3.880376     0.079392     105.89
 H      -5.813164     3.328539     0.296503      25.36
 H      -5.551317     4.947242     0.109369      25.23
 H      -4.009370     3.962902     0.672111      25.88
 C      -3.814506     2.441824    -3.231881      -9.05
 O      -3.765635     3.582329    -4.154265     181.35
 H      -3.615222     4.502056    -3.675815      21.42
 C      -3.403380     1.190284    -3.824713      54.77
 H      -2.977003     1.397776    -4.783707      25.62
 C      -3.965309     0.072034    -1.724822      22.32
 C      -4.031839    -1.138805    -0.737385     103.40
 H      -4.458625    -2.210529    -1.110712      25.39
 O      -4.720008    -0.794031     0.417767     174.31
 H      -4.042401    -0.314165     0.944072      28.21
 C      -2.558827    -1.689997    -0.698447      94.70
 H      -2.287315    -1.758312    -1.757874      26.97
 C      -2.572206    -3.114374    -0.137928     105.83
 O      -3.461886    -4.078835    -0.655683     211.99
 H      -3.192484    -4.206240    -1.583459      30.86
 H      -3.169626    -3.125948     0.907368      24.92
 H      -1.533657    -3.795410    -0.209612      24.47
 C       1.785354    -0.975355    -1.270523      49.09
 H       2.422387    -1.501629    -2.026717      24.89
 C       1.628834     0.502207     0.674186      64.89
 H       2.105207     1.375528     1.230102      22.63
 C       0.331470     0.141600     0.846475      21.09
 O      -0.525642     0.655283     1.808674     147.50
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 C      -0.618121     2.353724     1.980032      76.32
 H      -0.601811     2.553662     3.075966      25.21
 H       0.257502     2.834729     1.552901      26.52
 H      -1.593953     2.917460     1.773256      26.16
 C      -0.401457    -0.785935     0.018200       3.72
 O      -1.736181    -0.888260     0.132660     163.22
 C       0.400998    -1.241767    -1.130920      71.70
 H      -0.132650    -2.258081    -1.669359      21.52
 C       2.478278    -0.114480    -0.340473      19.54
 C       3.861361     0.372728    -0.730329      81.56
 H       3.970055    -0.149028    -1.787618      26.38
 O       4.014326     1.813013    -0.756518     210.10
 H       4.261562     2.354694     0.141911      22.31
 C       5.014089    -0.344739     0.173128     103.06
 H       4.855996    -0.118691     1.086530      31.56
 O       4.737323    -1.804269     0.176471     266.91
 H       4.533180    -2.072433    -0.702546      35.15
 C       6.461369    -0.071046    -0.273622     112.04
 O       6.953544     1.264766    -0.347654     207.29
 H       7.040192     1.510020     0.607440      29.95
 H       6.670855    -0.449683    -1.373603      29.95
 H       6.982711    -0.512540     0.436998      33.57
55
name= lig-ACN-Water-frame_548
 C      -3.519131     0.014172    -3.039167      59.86
 H      -3.230513    -0.874413    -3.638007      21.82
 C      -4.327710     1.350448    -1.157767      82.02
 H      -4.500490     1.408971     0.048423      20.08
 C      -4.331046     2.470695    -1.977220       8.01
 O      -4.873964     3.713867    -1.422366     217.34
 C      -5.023654     3.923443    -0.039844     110.95
 H      -5.510224     3.198918     0.563396      26.41
 H      -5.347486     5.053164     0.041515      25.17
 H      -3.998448     3.782946     0.445551      27.43
 C      -3.845251     2.454300    -3.294501       6.21
 O      -3.692862     3.638531    -4.145498     169.05
 H      -3.367657     4.448411    -3.556446      22.84
 C      -3.386183     1.233722    -3.866012      35.80
 H      -3.211780     1.034032    -4.955342      20.80
 C      -3.975681     0.148327    -1.725374      38.22
 C      -3.961008    -1.009218    -0.853043      75.69
 H      -4.842178    -1.596430    -1.490277      21.63
 O      -4.682924    -0.778117     0.474305      77.78
 H      -4.154752    -0.539378     1.219078      25.35
 C      -2.651898    -1.734088    -0.718716      88.84
 H      -2.149603    -1.841438    -1.679819      25.38
 C      -2.655968    -3.154753     0.000945     108.74
 O      -3.394252    -4.149363    -0.784791     254.13
 H      -3.021810    -4.262650    -1.620373      29.96
 H      -2.662869    -3.045428     1.206510      24.72
 H      -1.413683    -3.171528    -0.009640      23.85
 C       1.713941    -0.883892    -1.272347      55.60
 H       2.191688    -1.298275    -2.210615      26.97
 C       1.647192     0.542338     0.706962      38.82
 H       2.081244     1.240117     1.399701      22.00
 C       0.210071     0.197119     0.897634       3.50
 O      -0.601459     0.727192     1.936489     189.14
 C      -0.711432     2.187428     1.956543     103.30
 H      -0.764832     2.283595     2.994203      26.40
 H       0.279294     2.679195     1.559657      25.59
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 H      -1.521703     2.334330     1.133385      25.33
 C      -0.331408    -0.690779    -0.087179       9.31
 O      -1.745848    -0.896949     0.177233     129.44
 C       0.383310    -1.365398    -1.018482      73.92
 H      -0.210453    -1.944481    -1.975559      18.21
 C       2.387866    -0.042820    -0.345604      30.73
 C       3.885172     0.258423    -0.625397      91.56
 H       4.087690     0.124343    -1.752613      23.63
 O       4.046580     1.853411    -0.745198     183.32
 H       4.289778     1.980056     0.286852      22.62
 C       4.976500    -0.346399     0.150493     115.50
 H       4.966071     0.009319     1.031364      29.91
 O       4.700743    -1.776793     0.203708     261.59
 H       4.402691    -2.110498    -0.717123      28.72
 C       6.505925    -0.119297    -0.249997     100.78
 O       6.959321     1.280929    -0.357402     216.91
 H       6.882721     1.867122     0.460169      27.80
 H       6.640080    -0.632692    -1.345278      27.43
 H       7.055853    -0.734097     0.276908      31.84
55
name= lig-ACN-Water-frame_549
 C      -3.577027     0.124114    -3.086741      64.77
 H      -3.501319    -0.911784    -3.330832      24.82
 C      -4.286866     1.463186    -1.190858      65.89
 H      -4.737760     1.455824    -0.144071      18.52
 C      -4.328166     2.586999    -2.002414      16.74
 O      -4.897905     3.661342    -1.529116     229.02
 C      -4.948911     3.949965    -0.062586     111.05
 H      -5.818762     3.322585     0.241051      24.40
 H      -5.366975     5.017515     0.088160      24.56
 H      -3.926042     3.902147     0.337737      26.30
 C      -3.809950     2.507037    -3.425727      13.45
 O      -3.630906     3.642892    -4.095732     216.80
 H      -3.444527     4.456980    -3.543902      25.68
 C      -3.484857     1.233781    -3.848372      68.20
 H      -3.003344     1.184634    -4.901744      23.88
 C      -3.886420     0.250222    -1.722741      31.45
 C      -4.050992    -1.032438    -0.835273      61.86
 H      -4.742238    -1.972698    -1.312312      23.09
 O      -4.597026    -0.802045     0.487900     137.00
 H      -3.816538    -0.435297     1.010423      24.08
 C      -2.637372    -1.805370    -0.625527      77.42
 H      -2.246615    -1.915224    -1.653767      24.90
 C      -2.556246    -3.142916     0.044204     106.51
 O      -3.339251    -4.191536    -0.787620     186.74
 H      -2.965612    -4.182730    -1.754773      27.33
 H      -3.393988    -3.250438     0.894284      22.49
 H      -1.506162    -3.718721     0.153406      23.04
 C       1.693028    -0.872130    -1.229351      55.50
 H       2.234818    -1.135585    -2.174519      22.58
 C       1.563040     0.545198     0.788076      63.16
 H       2.055838     1.043043     1.521827      22.26
 C       0.211276     0.269464     0.887141       0.10
 O      -0.576418     0.695509     2.035976     234.77
 C      -0.807341     2.076593     1.889970     117.12
 H      -1.310467     2.617303     2.628095      27.42
 H       0.228130     2.653004     1.761796      23.67
 H      -1.558759     2.490143     1.084285      24.73
 C      -0.479496    -0.645162    -0.046960       2.04
 O      -1.765305    -0.893588     0.186795     158.35
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 C       0.384192    -1.377335    -1.002086      66.63
 H      -0.035135    -2.111794    -1.901080      16.36
 C       2.306007     0.023194    -0.383581      23.39
 C       3.836725     0.415299    -0.719514      77.72
 H       3.991334    -0.066041    -1.755132      25.66
 O       4.064793     1.766270    -0.657345     235.64
 H       4.460459     2.182906     0.190399      22.68
 C       4.988764    -0.378907     0.265541      93.82
 H       4.862771    -0.155274     1.177877      29.90
 O       4.691575    -1.768473     0.226418     261.31
 H       4.605956    -2.089325    -0.752296      28.84
 C       6.504404    -0.170962    -0.289044      97.88
 O       6.931032     1.236404    -0.351936     202.98
 H       6.783619     1.502327     0.577825      32.26
 H       6.664303    -0.463427    -1.474722      27.85
 H       7.101914    -0.619574     0.355430      31.68
55
name= lig-ACN-Water-frame_550
 C      -3.619209     0.098013    -3.081540      38.62
 H      -3.353168    -0.730398    -3.659671      24.97
 C      -4.258277     1.507545    -1.193269      63.36
 H      -4.747861     1.631711    -0.285602      21.75
 C      -4.303480     2.610473    -2.034923      20.52
 O      -4.946706     3.847513    -1.680155     179.77
 C      -4.934156     3.992362    -0.113143      97.37
 H      -5.674064     3.271588     0.505137      23.67
 H      -5.158434     5.059035    -0.186422      26.07
 H      -4.037860     3.743419     0.404824      27.52
 C      -3.796499     2.548786    -3.309862      13.50
 O      -3.565613     3.688664    -4.163036     232.17
 H      -3.549854     4.513781    -3.654840      24.14
 C      -3.527830     1.292144    -3.982975      34.97
 H      -3.012418     1.311374    -5.033898      19.23
 C      -3.876613     0.168359    -1.634642       7.83
 C      -3.978012    -1.136188    -0.747762      80.25
 H      -4.768797    -1.927237    -1.367826      22.39
 O      -4.529770    -0.829717     0.479628     195.36
 H      -3.985764    -0.240800     1.172014      20.50
 C      -2.545829    -1.790004    -0.634063      91.23
 H      -2.039632    -1.872479    -1.634888      25.87
 C      -2.671995    -3.308472     0.044998     110.40
 O      -3.274998    -4.191529    -0.775637     223.51
 H      -2.907522    -4.228885    -1.836058      22.85
 H      -3.165339    -3.053423     1.103643      24.36
 H      -1.589507    -3.541061     0.543914      25.67
 C       1.688017    -0.883736    -1.190383      78.73
 H       2.288602    -1.459696    -1.930706      19.77
 C       1.546976     0.512778     0.778788      44.51
 H       1.965139     1.145960     1.459404      25.11
 C       0.136250     0.200290     0.888726       5.40
 O      -0.496044     0.588098     2.069073      87.54
 C      -0.952142     2.254315     1.829336      64.45
 H      -1.526108     2.246977     2.666076      24.65
 H       0.079664     2.907244     2.051471      22.47
 H      -1.165177     2.096370     0.683760      22.81
 C      -0.466457    -0.692653    -0.002329      10.68
 O      -1.871526    -0.877130     0.202729     185.72
 C       0.290560    -1.253080    -0.992813      76.22
 H      -0.108119    -2.296727    -1.280431      20.70
 C       2.340025     0.130875    -0.339617      23.69
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 C       3.761713     0.387168    -0.655970      90.84
 H       3.983704     0.119637    -1.713919      27.41
 O       4.078113     1.812778    -0.670278     238.12
 H       4.336469     2.072523     0.273184      24.54
 C       4.948287    -0.389590     0.225601      95.03
 H       4.950390    -0.058076     1.115952      31.89
 O       4.701430    -1.830911     0.230087     258.41
 H       4.750464    -2.116085    -0.677424      31.42
 C       6.423736    -0.167406    -0.287317     107.85
 O       6.887614     1.176118    -0.306503     191.76
 H       7.114535     1.548085     0.583523      29.59
 H       6.462635    -0.775340    -1.385210      28.41
 H       6.996714    -0.806861     0.174014      33.11
55
name= lig-ACN-Water-frame_551
 C      -3.598087     0.135419    -3.115813      61.10
 H      -3.332715    -0.801194    -3.446228      25.09
 C      -4.278727     1.413946    -1.161644      51.08
 H      -4.448212     1.401681    -0.198031      21.41
 C      -4.333613     2.663340    -2.024316     -10.39
 O      -4.907902     3.958203    -1.677063     205.36
 C      -4.954221     4.126843    -0.254503     109.95
 H      -5.949001     3.513301     0.129380      24.07
 H      -4.987045     5.087495     0.214595      26.83
 H      -4.001643     3.759653    -0.061450      27.07
 C      -3.720461     2.605387    -3.445116      13.37
 O      -3.537585     3.672140    -4.234501     204.79
 H      -3.326591     4.532377    -3.792783      25.31
 C      -3.554822     1.307548    -3.852560      54.19
 H      -3.427840     1.102053    -4.958050      22.71
 C      -3.914135     0.159038    -1.764783      35.28
 C      -3.821669    -1.105790    -0.805788      66.68
 H      -4.693724    -1.897980    -1.300712      22.16
 O      -4.553052    -0.878907     0.552143     120.22
 H      -3.867938    -0.517373     1.212054      23.04
 C      -2.550900    -1.884747    -0.623370      88.18
 H      -2.029250    -1.952920    -1.636858      23.61
 C      -2.667220    -3.194947     0.119234     106.28
 O      -3.296983    -4.279683    -0.799106     143.37
 H      -2.682326    -4.201486    -1.670729      26.38
 H      -3.442383    -3.302498     0.939136      23.71
 H      -1.573901    -3.634424     0.231172      23.42
 C       1.651408    -0.900050    -1.089445      19.91
 H       2.194203    -1.567534    -1.777014      22.90
 C       1.527447     0.560370     0.720797      49.37
 H       1.841458     1.315702     1.426068      21.69
 C       0.208208     0.123010     0.997008       9.41
 O      -0.472238     0.695963     2.066889     204.48
 C      -0.988897     2.176885     1.844783      72.25
 H      -1.953935     2.368427     2.260629      25.34
 H      -0.209830     3.125861     2.163194      22.91
 H      -1.375878     2.357598     0.658646      24.21
 C      -0.529176    -0.682705     0.077631      11.75
 O      -1.854705    -0.860878     0.246669     145.17
 C       0.289115    -1.247720    -0.976568      73.33
 H       0.061380    -2.046049    -1.691340      22.26
 C       2.252064     0.021353    -0.326020      41.86
 C       3.818495     0.350667    -0.598987      91.09
 H       3.884794     0.024095    -1.612553      26.45
 O       4.064981     1.885922    -0.739659     236.85
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 H       4.476681     2.105878     0.108060      25.03
 C       4.858236    -0.401308     0.166705     115.27
 H       4.719807    -0.189366     1.089675      29.33
 O       4.724847    -1.877192     0.220689     272.19
 H       4.502477    -2.253924    -0.645099      29.98
 C       6.305900    -0.241620    -0.291122      98.54
 O       6.886616     1.138481    -0.286999     204.33
 H       7.074265     1.426485     0.677678      29.50
 H       6.414527    -0.248179    -1.515246      26.35
 H       6.821097    -0.863378     0.271053      31.66
55
name= lig-ACN-Water-frame_552
 C      -3.559968     0.084727    -3.121369      51.99
 H      -3.460866    -0.781479    -3.713201      26.12
 C      -4.317596     1.479251    -1.245790      76.45
 H      -4.539795     1.555659    -0.286239      24.73
 C      -4.324038     2.691647    -2.058621      29.12
 O      -4.789257     3.964205    -1.732985     227.62
 C      -4.928625     4.224833    -0.292462     116.12
 H      -5.970854     3.663769     0.168753      23.52
 H      -5.080459     5.249852    -0.412105      27.83
 H      -4.280794     3.841670     0.482772      26.29
 C      -3.794227     2.611829    -3.315588      12.77
 O      -3.505592     3.674251    -4.344026     213.33
 H      -3.498376     4.549787    -3.830730      23.86
 C      -3.532616     1.267446    -3.892652      43.75
 H      -3.279616     1.274711    -4.950116      19.72
 C      -3.918923     0.221869    -1.706032      31.48
 C      -3.965596    -1.050315    -0.845648      78.18
 H      -4.569085    -1.991109    -1.448727      22.69
 O      -4.513131    -0.956852     0.512022     149.84
 H      -3.959850    -0.466574     1.092965      27.42
 C      -2.576231    -1.806785    -0.573865      93.97
 H      -2.004815    -2.093600    -1.522925      25.21
 C      -2.673080    -3.251598     0.080451     115.70
 O      -3.294946    -4.289281    -0.754183     238.40
 H      -3.085863    -4.363596    -1.656244      29.34
 H      -3.221090    -3.045703     1.018538      26.41
 H      -1.651026    -3.524749     0.591572      25.58
 C       1.622823    -1.042507    -1.076102      34.04
 H       2.165478    -1.321719    -2.001878      23.13
 C       1.496462     0.654860     0.761673      31.90
 H       2.087930     1.511668     1.279391      20.40
 C       0.220991     0.182845     1.074860      17.43
 O      -0.513977     0.890176     2.090239     236.95
 C      -1.060978     2.081232     1.796548      93.78
 H      -1.975984     2.147985     2.429746      24.79
 H      -0.207731     2.857605     2.412704      22.86
 H      -0.900347     2.334840     0.568769      24.55
 C      -0.434555    -0.702628     0.113901       9.84
 O      -1.808740    -0.903858     0.308934     133.63
 C       0.245592    -1.321465    -0.947463      62.89
 H      -0.354819    -1.603536    -1.727009      22.57
 C       2.363728    -0.025010    -0.250386       7.51
 C       3.710598     0.393302    -0.754114      87.01
 H       3.934360     0.049087    -1.691561      27.09
 O       4.042767     1.811330    -0.789123     233.38
 H       4.460981     2.184031    -0.002311      25.68
 C       4.810828    -0.460895     0.265338      94.20
 H       4.814438    -0.163867     1.186935      27.52
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 O       4.683858    -1.908672     0.176633     264.11
 H       4.363456    -2.190565    -0.773905      25.78
 C       6.276185    -0.184181    -0.361952     100.48
 O       6.892098     1.104032    -0.221454     264.56
 H       6.924130     1.265076     0.748922      30.67
 H       6.248645    -0.805367    -1.415093      28.21
 H       6.879850    -0.857156     0.049729      31.55
55
name= lig-ACN-Water-frame_553
 C      -3.580069     0.118306    -3.106107      46.14
 H      -3.380683    -0.906554    -3.456424      27.40
 C      -4.368467     1.587302    -1.259495      77.01
 H      -4.897236     1.766903    -0.379952      24.47
 C      -4.277739     2.683408    -2.126022      21.41
 O      -4.632224     3.951180    -1.714234     183.76
 C      -4.999558     4.353624    -0.293705     110.16
 H      -6.127501     3.898896     0.019745      23.36
 H      -5.082271     5.440208    -0.282660      28.01
 H      -4.049865     4.199450     0.239113      26.84
 C      -3.773896     2.555261    -3.500108      20.33
 O      -3.533699     3.577788    -4.300913     155.75
 H      -3.503249     4.533178    -3.892833      21.66
 C      -3.474492     1.315163    -3.930673      59.40
 H      -2.995199     1.250773    -4.863763      25.12
 C      -3.922192     0.239672    -1.705264     -28.77
 C      -4.005299    -1.098177    -0.817446      57.40
 H      -4.908937    -1.684251    -1.450056      21.24
 O      -4.548517    -1.002900     0.441430     123.68
 H      -4.082174    -0.238611     0.897946      28.83
 C      -2.567938    -1.745213    -0.603608      71.74
 H      -2.150971    -1.535580    -1.640185      26.28
 C      -2.700512    -3.239165     0.104780     113.85
 O      -3.317296    -4.265144    -0.659997     227.21
 H      -3.051629    -4.051557    -1.539472      31.69
 H      -3.319876    -3.266817     0.951970      25.85
 H      -1.584078    -3.559715     0.246863      25.84
 C       1.675526    -1.048477    -1.073853      34.66
 H       2.084521    -1.412790    -2.032520      17.23
 C       1.621808     0.639667     0.760183      44.97
 H       1.919427     1.619132     1.386133      20.07
 C       0.220322     0.327935     1.042151      -8.49
 O      -0.510276     0.805335     2.113566     159.78
 C      -1.034468     2.250625     1.779425      78.22
 H      -2.202178     2.387259     2.016074      24.83
 H      -0.401327     3.283780     2.216830      22.52
 H      -1.254498     2.353291     0.522584      25.93
 C      -0.370139    -0.726085     0.247106       6.17
 O      -1.782895    -0.956572     0.386147     145.81
 C       0.256646    -1.300535    -0.880004      82.23
 H      -0.123034    -1.984845    -1.536273      25.18
 C       2.230617    -0.074328    -0.273733      36.22
 C       3.723879     0.295092    -0.726719      87.23
 H       3.688907     0.065636    -1.701722      28.75
 O       3.995438     1.725877    -0.836978     242.35
 H       4.236286     1.955125     0.164347      25.89
 C       4.845911    -0.449344     0.170072      98.88
 H       4.673473    -0.209464     1.114289      31.39
 O       4.585276    -1.891458     0.162791     253.38
 H       4.566737    -2.257765    -0.848785      27.78
 C       6.277086    -0.260837    -0.335812     102.85
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 O       6.868626     1.081602    -0.189463     224.10
 H       7.055641     1.348055     0.719746      31.71
 H       6.259166    -0.098404    -1.531783      28.33
 H       6.831322    -1.006708     0.034788      33.26
55
name= lig-ACN-Water-frame_554
 C      -3.577712     0.201901    -3.044936      58.90
 H      -3.105886    -0.774931    -3.389682      22.38
 C      -4.392973     1.536754    -1.282862      75.95
 H      -4.830477     1.593945    -0.251659      25.37
 C      -4.238120     2.666606    -2.145432       2.16
 O      -4.533037     4.054280    -1.705133     187.91
 C      -4.977336     4.463951    -0.387071     110.33
 H      -5.917122     3.750887     0.049087      23.50
 H      -5.184884     5.578059    -0.487209      27.26
 H      -4.285088     4.114770     0.476923      25.06
 C      -3.768239     2.504075    -3.522369      -5.65
 O      -3.555603     3.602021    -4.331135     147.73
 H      -3.418504     4.394519    -3.680452      21.35
 C      -3.368934     1.156964    -3.966655      58.19
 H      -3.012819     0.957167    -4.934925      26.42
 C      -4.020256     0.301655    -1.703308      38.10
 C      -3.946597    -1.032853    -0.863552      73.23
 H      -4.346277    -2.064799    -1.425056      23.94
 O      -4.685143    -0.951512     0.472175      70.28
 H      -4.091466    -0.488156     1.222830      23.70
 C      -2.586949    -1.763823    -0.617975      71.89
 H      -1.915030    -2.047423    -1.462991      25.62
 C      -2.624618    -3.111315     0.095671     111.00
 O      -3.388679    -4.221364    -0.661225     141.00
 H      -2.989149    -4.422810    -1.658779      24.39
 H      -2.926074    -2.906693     1.044769      28.53
 H      -1.572985    -3.467023     0.280456      27.13
 C       1.589763    -0.980457    -1.077327      24.16
 H       2.224762    -1.641193    -1.658834      18.57
 C       1.584600     0.596838     0.772691      51.20
 H       2.368588     1.289756     1.339133      20.01
 C       0.248054     0.306580     0.972739      10.19
 O      -0.542491     0.878304     2.106124     136.24
 C      -1.070529     2.373909     1.711629      62.25
 H      -2.132683     2.488606     2.357540      23.03
 H      -0.122045     3.084177     2.166258      21.46
 H      -0.905120     2.368920     0.442274      24.52
 C      -0.453330    -0.728783     0.254873       4.55
 O      -1.782631    -0.974772     0.480467     118.34
 C       0.353324    -1.354188    -0.774034      72.01
 H      -0.049928    -2.291741    -1.095491      22.28
 C       2.321021    -0.019313    -0.325080      43.14
 C       3.718574     0.186004    -0.699702     105.33
 H       3.905000    -0.246005    -1.618922      28.73
 O       3.935609     1.651086    -0.797162     230.32
 H       4.274636     2.119806     0.091409      24.77
 C       4.794965    -0.475918     0.060166     112.71
 H       4.863304    -0.078843     0.982419      28.73
 O       4.509993    -1.854985     0.192137     265.86
 H       4.423989    -2.313969    -0.781242      26.04
 C       6.309431    -0.228821    -0.379401     105.11
 O       6.871825     1.078546    -0.138489     252.32
 H       6.905665     1.260020     0.849074      31.29
 H       6.354104    -0.550897    -1.551558      30.31
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 H       6.842801    -1.000108    -0.035920      34.21
55
name= lig-ACN-Water-frame_555
 C      -3.472660     0.037086    -2.995996      40.49
 H      -3.198735    -1.048209    -3.337147      24.05
 C      -4.446499     1.582654    -1.243397      50.62
 H      -4.626240     1.801230    -0.080355      20.63
 C      -4.254136     2.722792    -2.078574      16.19
 O      -4.428091     4.069904    -1.796469     172.04
 C      -4.944127     4.408447    -0.453488     110.57
 H      -6.112179     3.984410    -0.447255      22.24
 H      -5.167946     5.579997    -0.535653      25.99
 H      -4.169343     4.252176     0.447931      22.92
 C      -3.717984     2.502760    -3.479110      14.94
 O      -3.565205     3.612439    -4.357989     190.70
 H      -3.570914     4.537716    -3.917109      23.70
 C      -3.380679     1.215405    -3.959836      31.90
 H      -2.993727     1.049185    -4.968113      20.45
 C      -4.044660     0.199972    -1.722305      17.33
 C      -3.911128    -1.008633    -0.792224      71.54
 H      -4.677415    -1.666943    -1.478116      23.65
 O      -4.742620    -0.871441     0.428311     131.21
 H      -4.111096    -0.808867     1.163977      27.12
 C      -2.488144    -1.691298    -0.534784      86.91
 H      -2.042281    -1.528094    -1.529645      25.06
 C      -2.601287    -3.133196     0.066106     118.80
 O      -3.431553    -4.099426    -0.626198     162.46
 H      -2.818200    -4.336695    -1.460801      27.55
 H      -3.164748    -3.151250     0.890429      27.75
 H      -1.561628    -3.446020     0.161829      26.30
 C       1.618645    -0.993801    -1.052605      43.26
 H       2.080844    -1.530899    -1.882315      21.45
 C       1.618662     0.566546     0.739980      35.41
 H       1.944487     1.204640     1.622146      19.80
 C       0.144677     0.286793     1.060793       0.34
 O      -0.563916     1.048004     1.988077     226.56
 C      -0.920434     2.310400     1.699861      96.45
 H      -2.042442     2.631275     2.243972      23.55
 H      -0.104282     3.175146     2.166565      22.41
 H      -1.299979     2.660600     0.495822      23.08
 C      -0.464549    -0.653790     0.183121       8.88
 O      -1.810036    -0.993715     0.499159     183.70
 C       0.275582    -1.517270    -0.613632      61.15
 H      -0.093417    -2.433406    -1.231301      20.50
 C       2.287810    -0.012460    -0.325682      31.68
 C       3.765658     0.260089    -0.775567      82.06
 H       3.751414     0.042295    -1.861378      24.42
 O       3.907542     1.646710    -0.759898     253.33
 H       4.483898     1.813669    -0.028677      26.67
 C       4.863899    -0.475095     0.181148      86.63
 H       4.754001    -0.151699     1.164747      27.10
 O       4.466380    -1.867338     0.273267     301.07
 H       4.359628    -2.166128    -0.717750      25.83
 C       6.320016    -0.263293    -0.459359     108.90
 O       6.875056     1.055884    -0.117137     254.23
 H       6.662814     1.201433     0.833701      32.47
 H       6.551091    -0.359335    -1.603880      28.81
 H       6.805806    -0.863114     0.100276      31.20
55
name= lig-ACN-Water-frame_556
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 C      -3.454361     0.047816    -3.047239      46.49
 H      -3.231810    -1.007580    -3.482036      24.99
 C      -4.385153     1.579897    -1.258569      63.59
 H      -4.794163     1.664641    -0.090477      19.63
 C      -4.206260     2.683223    -2.133994      43.69
 O      -4.352235     4.021811    -1.814901     215.86
 C      -4.978151     4.380725    -0.611489     107.97
 H      -6.005670     3.780286    -0.317665      22.76
 H      -4.814600     5.591200    -0.453853      24.30
 H      -4.320499     3.744355     0.188392      21.75
 C      -3.685086     2.552089    -3.430565      19.95
 O      -3.582001     3.523053    -4.363758     218.32
 H      -3.520014     4.402933    -3.882584      30.90
 C      -3.429483     1.211381    -3.787689      62.36
 H      -3.019430     1.248554    -4.837429      19.32
 C      -3.942600     0.267698    -1.688365      16.90
 C      -4.030322    -1.027245    -0.740781      97.20
 H      -4.403549    -2.087477    -1.238111      22.94
 O      -4.735784    -0.784969     0.418457     201.22
 H      -4.246796    -0.366000     1.127384      25.48
 C      -2.577343    -1.584258    -0.512209      73.51
 H      -1.989763    -1.540022    -1.407476      24.57
 C      -2.612147    -3.162562     0.081561     125.72
 O      -3.442939    -4.008729    -0.690280     225.45
 H      -3.159423    -4.180926    -1.523305      31.62
 H      -2.868993    -2.971644     1.050304      28.60
 H      -1.688837    -3.653017     0.257761      29.07
 C       1.551964    -1.160452    -0.994203      51.13
 H       1.909860    -1.423847    -1.969996      18.61
 C       1.517841     0.571111     0.836799      62.17
 H       2.056670     1.394316     1.217059      22.50
 C       0.192248     0.333014     0.982503      20.78
 O      -0.559475     1.028085     1.898962     177.08
 C      -0.859060     2.507103     1.663128      70.13
 H      -1.828298     2.597829     2.524353      20.63
 H       0.092363     3.251827     1.834566      21.19
 H      -1.122804     2.474316     0.379230      21.74
 C      -0.494506    -0.696548     0.273604       8.75
 O      -1.802599    -0.921761     0.523546     182.87
 C       0.332481    -1.526096    -0.607745      56.18
 H      -0.268801    -2.335190    -1.279157      19.48
 C       2.213459    -0.082661    -0.299853      26.82
 C       3.706760     0.308815    -0.725517      73.14
 H       4.026529    -0.173194    -1.750439      24.86
 O       3.978725     1.810216    -0.725231     208.22
 H       4.505101     2.148543     0.028502      25.91
 C       4.841137    -0.472681     0.124151      91.55
 H       4.881282     0.036053     1.065293      27.57
 O       4.475598    -1.866543     0.350998     286.44
 H       4.585561    -2.376741    -0.469841      31.18
 C       6.349300    -0.312350    -0.343005     108.87
 O       6.852157     1.042060    -0.128202     246.78
 H       6.790106     1.308020     0.793031      32.37
 H       6.229261    -0.380207    -1.488965      30.27
 H       6.911358    -1.066045    -0.259414      34.49
55
name= lig-ACN-Water-frame_557
 C      -3.533917     0.134060    -2.947301      70.17
 H      -3.152820    -0.796374    -3.459546      20.89
 C      -4.259912     1.510628    -1.301454      66.04
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 H      -4.964723     1.675754    -0.299761      22.45
 C      -4.133792     2.648001    -2.118636      23.52
 O      -4.357274     3.981366    -1.839054     218.78
 C      -4.952997     4.248059    -0.570845     109.09
 H      -6.121697     4.315731    -0.840841      24.75
 H      -4.831320     5.514721    -0.470496      25.52
 H      -4.570044     3.838302     0.481166      23.99
 C      -3.702316     2.464847    -3.390277      23.36
 O      -3.575655     3.457957    -4.369779     165.47
 H      -3.510915     4.342908    -3.963120      22.22
 C      -3.360568     1.225811    -3.872155      62.80
 H      -3.095859     0.910477    -4.926552      27.34
 C      -3.871543     0.201934    -1.654709      41.34
 C      -3.999859    -0.981102    -0.771367      65.49
 H      -4.773398    -1.689806    -1.378085      21.20
 O      -4.795935    -0.692686     0.525391     144.16
 H      -4.199555    -0.004075     0.995513      27.01
 C      -2.628481    -1.682475    -0.446061      78.44
 H      -2.206228    -1.689992    -1.418368      25.92
 C      -2.587579    -3.026291     0.098180     127.71
 O      -3.517118    -3.976336    -0.770762     148.98
 H      -3.237696    -3.792747    -1.707308      29.96
 H      -3.115108    -3.235516     0.958100      26.35
 H      -1.596508    -3.295184     0.005857      26.48
 C       1.616701    -1.182735    -0.955413      37.09
 H       2.177918    -1.844801    -1.613477      20.93
 C       1.610546     0.604975     0.715023      52.32
 H       1.992090     1.418244     1.125095      24.37
 C       0.170462     0.358856     0.926648     -13.57
 O      -0.606627     1.065213     1.907807     135.26
 C      -0.788598     2.560061     1.587890      79.37
 H      -1.577225     3.213093     2.398984      23.90
 H       0.250456     3.059675     1.812216      22.92
 H      -1.313244     2.906208     0.437749      24.79
 C      -0.416906    -0.817827     0.377790      11.70
 O      -1.846039    -0.788243     0.560234      81.34
 C       0.202902    -1.503649    -0.650451      91.00
 H      -0.313027    -2.447070    -1.181504      20.53
 C       2.276595    -0.121693    -0.250512      33.56
 C       3.671318     0.322829    -0.603987      66.38
 H       3.570323     0.305633    -1.804684      23.05
 O       4.030862     1.926425    -0.713878     145.78
 H       4.267106     2.120745     0.320258      24.51
 C       4.800437    -0.448657     0.207495      92.00
 H       4.691124    -0.107797     1.241782      27.38
 O       4.531716    -1.842204     0.401132     319.42
 H       4.571461    -2.200105    -0.477622      31.26
 C       6.270130    -0.302657    -0.378749     110.63
 O       6.854582     1.006166    -0.132191     202.34
 H       7.060298     1.133525     0.839578      30.38
 H       6.239534    -0.310453    -1.496989      29.43
 H       6.840897    -0.926513     0.074072      32.56
55
name= lig-ACN-Water-frame_558
 C      -3.445204     0.035528    -3.047975      59.15
 H      -3.277484    -1.009587    -3.245926      25.22
 C      -4.232537     1.533965    -1.183098      79.36
 H      -4.650960     1.701615    -0.074438      23.22
 C      -4.051711     2.595202    -2.091208       3.26
 O      -4.359159     3.902991    -1.773084     188.20
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 C      -5.060165     4.309911    -0.516279      95.63
 H      -6.185530     4.051860    -0.534049      24.47
 H      -4.529727     5.442865    -0.275713      23.95
 H      -4.729454     3.441887     0.220389      23.96
 C      -3.645020     2.410011    -3.567540       4.15
 O      -3.565392     3.459680    -4.378231     158.73
 H      -3.567629     4.338615    -3.941479      23.51
 C      -3.348679     1.093934    -3.950408      61.27
 H      -2.982150     1.036079    -5.001930      24.15
 C      -3.864560     0.271506    -1.606526       5.08
 C      -4.068125    -0.933217    -0.608685      93.52
 H      -4.753515    -1.752386    -1.150776      24.34
 O      -4.820994    -0.621920     0.513430     179.92
 H      -4.415033    -0.156178     1.353263      20.56
 C      -2.679340    -1.590897    -0.394898      90.73
 H      -2.078286    -1.594075    -1.248575      27.56
 C      -2.712258    -3.133207     0.070655     143.11
 O      -3.470586    -3.876715    -0.814076     166.48
 H      -3.304048    -3.793823    -1.911417      21.02
 H      -2.906759    -3.102458     1.160927      27.93
 H      -1.793786    -3.541686     0.143169      29.26
 C       1.630349    -1.229064    -0.856442      21.62
 H       2.201372    -1.945578    -1.478287      22.91
 C       1.533896     0.709867     0.623071      66.22
 H       1.940145     1.420146     1.171783      24.61
 C       0.195858     0.352965     1.015807       0.81
 O      -0.672483     1.192598     1.857745     188.82
 C      -0.654311     2.556977     1.556214      78.55
 H      -1.359779     2.920056     2.629455      22.40
 H       0.321402     3.022361     1.411881      24.94
 H      -1.243873     2.648044     0.370181      24.87
 C      -0.496119    -0.733536     0.390329      -3.07
 O      -1.916853    -0.747891     0.513004     105.92
 C       0.289464    -1.508184    -0.684873      64.54
 H      -0.078345    -2.410664    -1.263408      22.64
 C       2.305084    -0.109535    -0.220733      30.32
 C       3.735844     0.413101    -0.628172      70.07
 H       4.085806    -0.061142    -1.714446      22.45
 O       3.996937     1.886428    -0.599858     214.46
 H       4.364036     2.260758     0.335519      23.08
 C       4.768970    -0.365605     0.284356      95.10
 H       4.858365     0.096501     1.315710      26.45
 O       4.571008    -1.834351     0.381423     269.69
 H       4.590707    -2.283596    -0.528486      28.06
 C       6.183608    -0.234657    -0.361543     116.49
 O       6.890523     1.016031    -0.136622     235.08
 H       7.092692     0.967560     0.831374      32.40
 H       6.321261    -0.619739    -1.363465      32.74
 H       6.605055    -1.005252     0.066585      34.07
55
name= lig-ACN-Water-frame_559
 C      -3.400252    -0.086572    -2.982550      52.41
 H      -3.201206    -1.001781    -3.406060      24.69
 C      -4.144036     1.591366    -1.155560      55.66
 H      -4.307393     1.741361    -0.074358      19.48
 C      -4.036566     2.578874    -2.140123      15.66
 O      -4.376310     3.912669    -1.725684     205.78
 C      -5.077207     4.205551    -0.483783      98.24
 H      -6.151642     4.454034    -0.641953      24.46
 H      -4.732467     5.409704    -0.114746      23.42
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 H      -4.766252     3.665498     0.537443      23.35
 C      -3.625760     2.338791    -3.463411      28.72
 O      -3.550280     3.487832    -4.442131     277.74
 H      -3.331326     4.306227    -3.897282      27.50
 C      -3.337464     0.973786    -3.978967      36.71
 H      -2.932399     0.734476    -4.955146      17.67
 C      -3.888676     0.237762    -1.668561      13.64
 C      -4.060339    -0.906789    -0.590837      70.47
 H      -4.565864    -1.825227    -1.093520      23.69
 O      -4.931144    -0.556772     0.568720     207.67
 H      -4.315041    -0.404227     1.329335      23.18
 C      -2.664185    -1.549998    -0.359661      84.36
 H      -2.407499    -1.500027    -1.383825      28.33
 C      -2.703387    -3.112657     0.130063     114.27
 O      -3.519303    -3.856142    -0.894410     153.45
 H      -2.835646    -3.820270    -1.699130      26.91
 H      -3.564062    -3.284072     0.842563      24.14
 H      -1.807847    -3.510434     0.201135      28.37
 C       1.721776    -1.226406    -0.743207      45.43
 H       2.209642    -1.695156    -1.645002      18.87
 C       1.445586     0.780051     0.668945      43.01
 H       1.910530     1.698526     0.906778      19.63
 C       0.096795     0.350893     1.042395      16.80
 O      -0.630647     1.162984     1.801135     200.91
 C      -0.576719     2.594212     1.488341      79.61
 H      -1.039916     3.364976     2.460351      22.53
 H       0.412223     2.945624     1.344898      24.53
 H      -1.402354     2.915121     0.525106      23.07
 C      -0.522078    -0.621561     0.206719       9.60
 O      -1.917088    -0.735356     0.508730     172.50
 C       0.298896    -1.448648    -0.499539      73.88
 H      -0.230163    -2.129006    -1.091879      24.63
 C       2.265301     0.009699    -0.282253      11.73
 C       3.791898     0.384029    -0.571857      76.59
 H       3.973610     0.160837    -1.799611      22.41
 O       3.921259     1.788404    -0.482098     262.75
 H       4.453481     1.959541     0.305199      26.47
 C       4.825862    -0.314407     0.278339      98.00
 H       4.638091    -0.002797     1.407149      25.32
 O       4.565095    -1.768222     0.354341     317.20
 H       4.779311    -2.090402    -0.637542      28.08
 C       6.230984    -0.255279    -0.246056     108.15
 O       6.929352     1.030543    -0.154399     258.99
 H       7.129966     1.336360     0.730814      33.56
 H       5.994812    -0.200741    -1.337878      30.95
 H       6.856933    -0.915650     0.069085      33.02
55
name= lig-ACN-Water-frame_560
 C      -3.461338    -0.080039    -2.932936      53.23
 H      -3.190603    -1.039438    -3.078561      24.15
 C      -3.995020     1.478008    -1.294353      71.49
 H      -4.327712     1.656983    -0.350953      21.87
 C      -4.079461     2.649754    -2.109398      21.01
 O      -4.349673     3.941031    -1.732097     213.66
 C      -5.081135     4.199477    -0.445315      98.96
 H      -6.087497     3.998591    -0.715203      27.01
 H      -4.595479     5.383099    -0.326753      22.58
 H      -4.980039     3.371630     0.374868      22.39
 C      -3.600329     2.365638    -3.517227      14.71
 O      -3.519425     3.339424    -4.394417     187.25
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 H      -3.317988     4.293459    -4.076634      22.91
 C      -3.313988     1.001738    -3.811992      47.20
 H      -3.097499     0.811532    -4.825055      25.90
 C      -3.898742     0.164612    -1.603869      36.62
 C      -4.101663    -0.929218    -0.634944      82.96
 H      -4.818495    -1.586962    -1.165647      22.66
 O      -4.988511    -0.528366     0.579290     202.14
 H      -4.485583    -0.236674     1.348166      25.00
 C      -2.718115    -1.637208    -0.350469      80.94
 H      -2.049598    -1.805996    -1.187940      23.07
 C      -2.828449    -2.999429     0.167625     106.32
 O      -3.488171    -3.847242    -0.999453     176.87
 H      -3.092420    -4.028847    -1.835200      27.56
 H      -3.266658    -3.065698     1.247763      24.60
 H      -1.963696    -3.341781     0.459942      28.57
 C       1.670577    -1.102137    -0.706931      67.12
 H       2.255407    -1.880543    -1.299008      17.43
 C       1.508527     0.778208     0.634142      60.99
 H       1.728227     1.752928     1.234797      17.59
 C       0.130685     0.492553     0.873613       2.01
 O      -0.675864     1.201378     1.853036     168.53
 C      -0.554472     2.695290     1.439402      73.65
 H      -0.752443     3.167995     2.638456      20.23
 H       0.454536     2.885830     1.043702      22.01
 H      -1.328657     2.924407     0.433542      21.91
 C      -0.524670    -0.529675     0.229101      12.65
 O      -1.833590    -0.722539     0.502440     167.91
 C       0.329612    -1.471861    -0.472682      75.54
 H       0.033795    -2.308627    -0.936707      20.95
 C       2.236358     0.058829    -0.210572      52.32
 C       3.656308     0.361415    -0.537877      72.23
 H       3.820443     0.052725    -1.740360      21.36
 O       3.887536     1.785102    -0.376846     318.46
 H       4.136030     2.149917     0.459863      26.43
 C       4.833289    -0.412659     0.368592      77.59
 H       4.736368     0.066286     1.488853      24.33
 O       4.549005    -1.723791     0.305452     327.55
 H       4.743979    -2.176168    -0.606983      26.16
 C       6.367337    -0.166890    -0.230660     100.29
 O       6.990087     1.116447    -0.161460     231.89
 H       6.943357     1.457733     0.774744      31.94
 H       6.396001    -0.490897    -1.352007      30.50
 H       6.811898    -0.989895     0.139422      33.26
55
name= lig-ACN-Water-frame_561
 C      -3.507889    -0.095905    -2.917367      18.42
 H      -3.335603    -0.965028    -3.461146      21.02
 C      -4.046841     1.572799    -1.212775      65.50
 H      -4.353432     1.682987    -0.307718      23.16
 C      -4.009442     2.580052    -2.148674      32.96
 O      -4.287310     3.953650    -1.744027     220.04
 C      -5.093069     4.158102    -0.522696     107.74
 H      -6.155769     4.143853    -0.561583      26.88
 H      -4.999677     5.221582     0.163966      24.75
 H      -4.533323     3.533440     0.232250      24.39
 C      -3.629886     2.352919    -3.378511      25.19
 O      -3.455492     3.260725    -4.454333     236.95
 H      -3.479016     4.185410    -4.016846      26.15
 C      -3.295450     1.044138    -3.726084      92.39
 H      -2.880833     0.929430    -4.702077      24.37
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 C      -3.850495     0.159576    -1.608627       6.59
 C      -4.202201    -0.967699    -0.582087      87.55
 H      -4.653347    -1.821367    -1.004267      25.03
 O      -4.959816    -0.539569     0.502328     260.12
 H      -4.329372    -0.358614     1.192885      27.18
 C      -2.697442    -1.601286    -0.363620      61.89
 H      -2.362259    -1.605811    -1.446806      22.43
 C      -2.922738    -3.083261     0.172918     121.45
 O      -3.487053    -3.809080    -0.867235     231.81
 H      -3.017439    -3.500653    -1.599481      33.03
 H      -3.835306    -3.122030     0.893046      23.33
 H      -2.042354    -3.476108     0.351082      28.97
 C       1.607545    -1.106730    -0.752648      14.77
 H       2.350017    -1.849962    -1.142373      15.48
 C       1.468799     0.940706     0.725546      45.40
 H       2.345480     1.483708     1.405156      15.20
 C       0.085586     0.655360     0.821625       7.35
 O      -0.649878     1.353113     1.800898     203.06
 C      -0.574613     2.687498     1.483296     101.42
 H      -0.709947     3.540231     2.441021      21.79
 H       0.384235     3.046858     0.952056      22.30
 H      -1.585913     2.997935     0.786580      23.19
 C      -0.484313    -0.609571     0.245715      -5.64
 O      -1.878065    -0.754771     0.496495     204.44
 C       0.309730    -1.474112    -0.520893      60.79
 H      -0.044294    -2.438660    -0.620541      19.26
 C       2.280948    -0.004584    -0.127495      31.78
 C       3.706579     0.421193    -0.405596      90.03
 H       3.984329     0.139911    -1.567441      20.75
 O       3.859685     1.863142    -0.361750     267.39
 H       4.088769     2.028138     0.616157      25.30
 C       4.821251    -0.313804     0.270287      90.21
 H       4.944624    -0.209870     1.479989      22.54
 O       4.540770    -1.856021     0.298651     308.73
 H       4.766710    -2.159516    -0.605843      28.15
 C       6.404744    -0.159153    -0.201980     104.73
 O       7.054643     1.208564    -0.160125     221.50
 H       6.827801     1.594991     0.726326      32.70
 H       6.516845    -0.555026    -1.228964      30.92
 H       6.972801    -0.507885     0.535719      31.14
55
name= lig-ACN-Water-frame_562
 C      -3.508672    -0.049664    -2.944023      46.31
 H      -3.274915    -1.128152    -3.205368      20.83
 C      -4.168715     1.512876    -1.044578      61.36
 H      -4.420665     1.683521    -0.082071      21.57
 C      -3.999937     2.671360    -1.965167      -1.39
 O      -4.256497     4.001768    -1.752569     196.43
 C      -5.033168     4.113093    -0.524891     108.82
 H      -5.949686     3.706581    -0.884869      26.73
 H      -4.833937     5.318894    -0.601394      23.11
 H      -4.840575     3.518199     0.385707      25.18
 C      -3.564501     2.338262    -3.455905       5.23
 O      -3.403176     3.246383    -4.475318     166.79
 H      -3.366128     4.196532    -4.273978      23.04
 C      -3.237719     1.016395    -3.820433      47.17
 H      -2.779575     0.817200    -4.805251      26.89
 C      -3.949531     0.218075    -1.565004      26.77
 C      -4.098132    -0.970743    -0.652115      88.33
 H      -4.692994    -1.601381    -1.191256      25.82
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 O      -4.921317    -0.564625     0.502493     183.77
 H      -4.437018    -0.374079     1.347783      23.65
 C      -2.763928    -1.603042    -0.316092      78.47
 H      -2.181064    -1.700339    -1.329158      21.54
 C      -2.929956    -3.058610     0.263033     126.60
 O      -3.549467    -3.851924    -0.794370     155.35
 H      -3.307641    -3.840594    -1.825637      22.38
 H      -3.581364    -2.980668     1.224991      25.29
 H      -2.217316    -3.485028     0.804482      27.75
 C       1.713258    -1.150643    -0.740445      76.98
 H       2.210746    -1.692791    -1.555435      16.18
 C       1.489394     0.842340     0.737532      31.44
 H       1.637692     1.941161     1.392775      12.22
 C       0.086779     0.622151     0.853065      11.50
 O      -0.617408     1.424953     1.728978     197.03
 C      -0.701683     2.915207     1.516701      81.02
 H      -0.665119     3.213866     2.679371      20.26
 H       0.290667     3.226639     0.850922      20.72
 H      -1.681037     3.187487     0.801578      22.43
 C      -0.529902    -0.520347     0.288833      11.16
 O      -1.901295    -0.791396     0.491650     178.68
 C       0.244056    -1.458584    -0.483837      81.14
 H      -0.227749    -2.341799    -0.991591      19.92
 C       2.223802     0.041354    -0.045315      37.61
 C       3.783094     0.467118    -0.428130      71.21
 H       3.707219     0.305922    -1.587464      22.76
 O       3.865264     1.928647    -0.342200     240.83
 H       4.422364     2.473267     0.384510      23.65
 C       4.958018    -0.406159     0.288783      63.57
 H       4.679401     0.035601     1.412957      22.25
 O       4.575690    -1.858542     0.272365     351.91
 H       4.861713    -2.234511    -0.559598      32.08
 C       6.407465    -0.134452    -0.074947     109.28
 O       7.026320     1.286863    -0.191995     209.78
 H       6.998934     1.820990     0.622937      32.24
 H       6.708722    -0.485016    -0.997992      33.14
 H       6.843438    -0.915493     0.516393      32.19
55
name= lig-ACN-Water-frame_563
 C      -3.499850     0.039708    -2.855585      57.84
 H      -3.119397    -1.066271    -2.996644      19.40
 C      -4.238045     1.589615    -1.096416      62.75
 H      -4.565066     1.567886    -0.048659      22.48
 C      -3.920999     2.566807    -2.065792       8.89
 O      -4.156621     3.959108    -1.725533     212.04
 C      -5.064390     4.210005    -0.589332     103.62
 H      -6.050388     3.679534    -0.568397      26.48
 H      -5.483459     5.271052    -0.260797      25.11
 H      -4.445104     3.962203     0.246181      27.89
 C      -3.495452     2.338534    -3.373588      26.96
 O      -3.363410     3.278488    -4.462023     180.70
 H      -3.179681     4.167283    -4.108120      25.26
 C      -3.219521     0.995839    -3.847950      73.39
 H      -2.952304     0.818417    -4.934363      25.17
 C      -4.006032     0.300537    -1.610903      25.77
 C      -4.071546    -0.913092    -0.688487      70.39
 H      -4.553756    -1.675987    -1.097772      26.75
 O      -4.911486    -0.648983     0.531513     126.09
 H      -4.268240    -0.171191     1.208082      24.03
 C      -2.683583    -1.697947    -0.333877      67.91
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 H      -2.072387    -2.031745    -1.297900      25.30
 C      -2.941330    -2.982758     0.383374     110.85
 O      -3.661725    -3.970789    -0.699615      69.14
 H      -2.854563    -3.791605    -1.409610      28.15
 H      -3.778807    -2.961611     1.082824      24.89
 H      -1.982922    -3.286236     0.451916      27.67
 C       1.636952    -1.073573    -0.628002      39.04
 H       2.113423    -1.578972    -1.429258      23.56
 C       1.414803     0.759778     0.751613      35.15
 H       1.995759     1.888354     0.937975      17.17
 C       0.054757     0.545839     0.936998      14.61
 O      -0.698042     1.507979     1.686118     188.03
 C      -0.776799     3.021863     1.524772      87.91
 H      -0.704912     3.473873     2.577295      24.87
 H       0.036159     3.723552     0.893295      23.59
 H      -1.889428     3.318953     1.160639      24.81
 C      -0.576063    -0.555525     0.249762      11.30
 O      -1.926355    -0.743379     0.575132     131.52
 C       0.337923    -1.340199    -0.466842      68.43
 H      -0.103444    -2.010913    -1.320695      21.77
 C       2.373310    -0.011018    -0.107738      27.08
 C       3.721311     0.488533    -0.520781      82.86
 H       4.039043     0.195142    -1.571868      22.45
 O       3.916996     1.969427    -0.374339     276.82
 H       4.292797     1.993880     0.603890      22.39
 C       4.883751    -0.385858     0.376842      86.72
 H       4.903006    -0.273808     1.635882      23.17
 O       4.671500    -1.751767     0.252830     324.77
 H       4.825357    -2.069526    -0.644969      30.08
 C       6.511789    -0.135592    -0.021879     104.08
 O       6.906188     1.257056    -0.167051     198.35
 H       6.965960     1.596833     0.750404      32.16
 H       6.500898    -0.451331    -0.962381      34.84
 H       7.283375    -0.459351     0.702864      30.73
55
name= lig-ACN-Water-frame_564
 C      -3.420121     0.000978    -2.843139      65.14
 H      -3.301867    -1.076610    -3.369749      25.43
 C      -4.265661     1.606271    -1.250502      61.13
 H      -4.745867     2.185059    -0.363895      16.65
 C      -3.922203     2.674788    -2.123390      15.06
 O      -4.092329     3.955894    -1.735449     182.80
 C      -5.057423     4.273066    -0.569701     101.83
 H      -5.838866     3.444220    -0.584661      26.28
 H      -5.186396     5.267387    -1.050935      24.42
 H      -4.571441     4.263069     0.413820      25.91
 C      -3.396487     2.364123    -3.445196      38.30
 O      -3.332000     3.321845    -4.349746     196.85
 H      -3.164015     4.263622    -3.998974      25.43
 C      -3.264489     1.048220    -3.763826      25.81
 H      -2.889231     0.751704    -4.795495      17.29
 C      -3.976879     0.264473    -1.559926      37.60
 C      -4.106693    -0.959196    -0.660947     100.25
 H      -4.616194    -1.596315    -1.214201      26.06
 O      -4.850413    -0.759477     0.514187     216.88
 H      -4.391238    -0.183852     1.237221      21.53
 C      -2.711349    -1.587243    -0.332375      60.35
 H      -2.131505    -1.565741    -1.365037      21.12
 C      -3.007013    -3.083704     0.371951     123.31
 O      -3.611429    -3.979378    -0.519657     212.05
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 H      -3.199640    -4.213134    -1.351935      28.41
 H      -3.472866    -2.981446     1.323163      25.50
 H      -2.230852    -3.597852     0.904111      26.97
 C       1.722824    -1.076003    -0.712375      21.01
 H       2.272993    -1.832723    -1.200550      17.16
 C       1.499023     0.806907     0.699009      58.20
 H       1.899392     1.761836     1.424106      18.18
 C       0.080233     0.629957     0.980079      -7.82
 O      -0.816321     1.565350     1.643642     169.06
 C      -0.861983     3.038083     1.568921      95.48
 H      -0.659676     3.366493     2.567485      23.38
 H      -0.051780     3.252663     0.619502      20.56
 H      -1.919789     3.182401     1.132953      21.08
 C      -0.568167    -0.524927     0.383487       1.95
 O      -1.929615    -0.762574     0.555085     158.62
 C       0.244731    -1.278053    -0.543164      76.01
 H      -0.126799    -2.301539    -1.081601      18.94
 C       2.322712     0.056932    -0.074020      26.42
 C       3.845675     0.463807    -0.442288      79.93
 H       3.901955     0.223067    -1.520213      22.39
 O       3.953658     1.868734    -0.425722     293.94
 H       4.141342     2.371410     0.396711      24.40
 C       4.927999    -0.271624     0.436628      76.82
 H       4.501406     0.102635     1.584448      20.76
 O       4.730086    -1.712814     0.244146     324.75
 H       4.895298    -1.854170    -0.739963      26.57
 C       6.475026    -0.101736    -0.011078     109.02
 O       6.776072     1.262201    -0.118139     256.49
 H       6.696272     1.817160     0.713304      29.54
 H       6.806421    -0.652741    -0.776291      33.77
 H       6.986397    -0.821060     0.768940      29.96
55
name= lig-ACN-Water-frame_565
 C      -3.419071    -0.045284    -2.854779      35.56
 H      -3.236410    -1.199704    -3.107901      22.11
 C      -4.262029     1.599341    -1.343721      64.80
 H      -4.723926     1.463098    -0.244748      20.97
 C      -3.938827     2.681000    -2.126354      22.37
 O      -4.050939     4.049676    -1.721991     238.54
 C      -4.957802     4.341252    -0.695108     128.21
 H      -5.927385     3.698865    -0.582202      25.73
 H      -5.592061     5.248482    -0.910128      26.85
 H      -4.573390     4.665236     0.258547      27.93
 C      -3.400641     2.443942    -3.388834      16.38
 O      -3.260458     3.448763    -4.368619     201.53
 H      -3.155412     4.441858    -3.998712      22.59
 C      -3.196902     1.026045    -3.763927      67.92
 H      -2.846606     0.873558    -4.811894      24.77
 C      -3.896625     0.233900    -1.560154      18.18
 C      -4.116249    -0.993979    -0.637947     102.72
 H      -4.525341    -1.751506    -1.132140      28.41
 O      -4.887575    -0.847372     0.554259     207.44
 H      -4.296993    -0.566387     1.273667      25.13
 C      -2.738247    -1.631003    -0.308535      69.96
 H      -2.204542    -1.879600    -1.317802      24.07
 C      -2.903221    -3.035521     0.400930     115.57
 O      -3.649848    -4.052672    -0.395358     159.79
 H      -3.174186    -3.995948    -1.169964      34.62
 H      -3.721616    -2.805552     0.946608      26.04
 H      -1.903329    -3.335043     0.718400      27.46
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 C       1.644012    -1.088953    -0.759726      21.66
 H       2.274649    -1.744893    -1.346595      19.55
 C       1.461272     1.013350     0.828979      38.50
 H       2.044701     1.876178     1.462428      18.78
 C       0.060983     0.757124     0.926740      -2.36
 O      -0.905261     1.470220     1.641138     207.07
 C      -0.885083     2.915824     1.511249     111.81
 H      -0.517030     3.401568     2.358244      26.81
 H      -0.086593     3.356681     0.627072      22.81
 H      -1.811658     3.295391     1.185592      26.28
 C      -0.459397    -0.481410     0.373542      -8.82
 O      -1.903172    -0.737339     0.566813      95.33
 C       0.284437    -1.282748    -0.526898      73.53
 H      -0.331054    -2.261122    -0.758699      19.99
 C       2.305110     0.051820    -0.086826      -1.85
 C       3.845957     0.406998    -0.353158      96.93
 H       4.044968     0.009529    -1.342590      25.01
 O       3.995027     1.871211    -0.490103     238.27
 H       4.347602     2.080906     0.335876      25.68
 C       4.946013    -0.277445     0.356282     105.00
 H       5.090352    -0.028147     1.618683      20.95
 O       4.740210    -1.676907     0.304263     286.33
 H       4.924982    -2.090376    -0.660449      26.40
 C       6.332815    -0.100762     0.119411     104.79
 O       6.734036     1.358592    -0.100517     238.13
 H       6.583871     1.749434     0.781957      30.78
 H       6.485089    -0.397354    -0.836741      32.50
 H       6.933293    -0.416424     1.080037      29.07
55
name= lig-ACN-Water-frame_566
 C      -3.382826    -0.013262    -2.939744      62.78
 H      -2.931878    -0.996494    -3.288670      19.73
 C      -4.262347     1.503228    -1.179510      52.88
 H      -4.725349     1.903201    -0.158993      21.04
 C      -3.952029     2.680854    -2.054062     -16.84
 O      -4.008004     4.096324    -1.763389     210.07
 C      -5.016125     4.512785    -0.750899     117.66
 H      -5.535365     3.516244    -0.501157      24.61
 H      -5.359069     5.437300    -1.067231      27.91
 H      -4.360569     4.508801     0.084310      28.08
 C      -3.421521     2.420707    -3.423152       1.03
 O      -3.210848     3.461455    -4.389543     162.02
 H      -2.998183     4.384079    -3.911170      20.30
 C      -3.097713     1.097204    -3.776142      59.92
 H      -2.758022     0.856042    -4.764891      29.16
 C      -3.884847     0.203208    -1.658010      32.94
 C      -4.052971    -1.029986    -0.637563      79.65
 H      -4.628951    -1.649601    -1.188227      25.81
 O      -4.931945    -0.879141     0.618581     141.62
 H      -4.447772    -0.590774     1.378284      26.38
 C      -2.656227    -1.711174    -0.335164      66.79
 H      -2.075875    -1.867996    -1.284145      22.72
 C      -2.895698    -2.921009     0.532603     107.51
 O      -3.611175    -4.094257    -0.347550      99.22
 H      -3.399722    -4.125340    -1.392277      25.86
 H      -3.137692    -2.879235     1.477414      27.47
 H      -1.896652    -3.424667     0.740915      25.48
 C       1.635304    -0.933083    -0.667737      54.18
 H       2.065106    -1.450698    -1.561368      20.87
 C       1.474580     0.988271     0.787299      60.62
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 H       1.951196     1.981600     1.069919      19.57
 C       0.048113     0.755775     0.878200       0.48
 O      -0.944493     1.381076     1.635611     191.91
 C      -0.851822     2.856338     1.437409     108.78
 H      -0.634610     3.248993     2.383500      26.22
 H      -0.089256     3.027040     0.479526      23.60
 H      -1.803863     3.091140     1.209852      27.57
 C      -0.500329    -0.418700     0.258513      -2.10
 O      -1.816248    -0.696607     0.575552      89.42
 C       0.322202    -1.365762    -0.404494      62.35
 H      -0.004486    -2.147796    -1.127238      20.42
 C       2.215293     0.136011    -0.002543      32.49
 C       3.679242     0.401246    -0.464273      77.19
 H       3.811614     0.069893    -1.455155      24.81
 O       4.036455     1.862205    -0.507822     225.08
 H       4.349537     2.330839     0.312346      23.19
 C       4.831661    -0.362218     0.577140      52.06
 H       4.307073    -0.131174     1.727181      21.24
 O       4.709633    -1.765767     0.394462     288.74
 H       4.919047    -1.882636    -0.668818      24.13
 C       6.431560     0.088447     0.066349      98.42
 O       6.693323     1.439348    -0.048023     272.91
 H       7.076683     1.913347     0.721373      28.71
 H       6.719278    -0.561753    -0.736770      32.77
 H       7.228542    -0.530606     0.790131      28.65
55
name= lig-ACN-Water-frame_567
 C      -3.285867     0.066504    -2.971470      42.35
 H      -3.090992    -0.915508    -3.366918      26.94
 C      -4.178439     1.613325    -1.160279      54.62
 H      -4.555827     1.601923    -0.081745      19.89
 C      -3.918709     2.652124    -2.069082      25.58
 O      -4.015263     4.026786    -1.849071     201.65
 C      -4.924977     4.557165    -0.727880     129.30
 H      -5.976201     4.139966    -0.661161      26.29
 H      -5.368967     5.366210    -1.214831      28.91
 H      -4.634588     5.038428     0.169855      27.88
 C      -3.439870     2.436889    -3.393325      25.07
 O      -3.193363     3.360406    -4.329178     202.00
 H      -3.135214     4.326681    -4.000111      23.10
 C      -3.051384     1.169828    -3.827879      19.86
 H      -2.535755     1.118927    -4.741177      19.88
 C      -3.945330     0.192211    -1.585346       6.77
 C      -4.030628    -1.029036    -0.655006      91.99
 H      -4.475217    -1.886716    -1.080924      27.65
 O      -4.850393    -0.863844     0.574609     167.38
 H      -4.428584    -0.224815     1.253696      23.58
 C      -2.633004    -1.625295    -0.253127      86.39
 H      -2.108495    -1.888680    -1.162012      25.69
 C      -2.779148    -3.092859     0.531958     110.12
 O      -3.571625    -4.016284    -0.215821     151.96
 H      -3.203431    -3.685045    -1.161343      29.47
 H      -3.474388    -2.862697     1.191932      26.47
 H      -1.690302    -3.503864     0.688510      24.98
 C       1.657766    -0.881897    -0.623102      68.94
 H       2.410175    -1.398291    -1.319032      17.97
 C       1.363098     1.018085     0.745236      61.84
 H       1.670175     1.912332     1.220099      21.85
 C       0.027823     0.604610     0.866320      16.48
 O      -0.884381     1.370917     1.600938     220.95
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 C      -0.896626     2.795087     1.427710     119.93
 H      -0.496800     3.306771     2.200479      27.85
 H      -0.069865     3.114798     0.581137      24.40
 H      -1.757596     3.153195     1.041797      27.39
 C      -0.523487    -0.483667     0.224676      14.37
 O      -1.873971    -0.727753     0.529127     176.59
 C       0.338990    -1.367081    -0.409099      68.91
 H      -0.034665    -2.191937    -0.930041      22.90
 C       2.263905     0.240113    -0.037357      31.28
 C       3.669067     0.478069    -0.410250     100.81
 H       3.745792     0.117310    -1.383738      22.85
 O       4.006470     1.850887    -0.531704     256.83
 H       4.287228     2.043179     0.471741      20.79
 C       4.684915    -0.379647     0.577299      56.48
 H       4.548636    -0.000527     1.806940      20.56
 O       4.681745    -1.872896     0.477252     268.73
 H       4.807790    -2.111719    -0.549673      25.81
 C       6.430754     0.124396     0.134430      69.88
 O       6.701581     1.576587    -0.023779     232.35
 H       7.254914     1.859078     0.767750      28.61
 H       6.302226    -0.082448    -0.928709      29.86
 H       7.054233    -0.329410     1.084922      27.55
55
name= lig-ACN-Water-frame_568
 C      -3.303683     0.078275    -2.853427      68.04
 H      -3.109724    -0.873439    -3.126969      24.43
 C      -4.071464     1.569997    -1.192104      89.36
 H      -4.419663     1.937478    -0.252201      19.42
 C      -3.906067     2.653594    -2.070387      18.05
 O      -4.095211     3.992488    -1.784432     299.98
 C      -4.915510     4.682676    -0.877136     119.31
 H      -5.665117     3.906783    -0.519878      27.23
 H      -4.991697     5.653649    -1.211654      27.47
 H      -4.205007     4.580029    -0.049902      26.39
 C      -3.411963     2.407260    -3.339387      30.60
 O      -3.177701     3.394621    -4.312301     236.10
 H      -3.294068     4.255894    -3.900790      27.04
 C      -3.025767     1.106243    -3.770824      45.53
 H      -2.622016     0.997331    -4.749747      22.11
 C      -3.860987     0.285237    -1.672774      39.47
 C      -4.004613    -1.041313    -0.638524      80.57
 H      -4.560038    -1.720057    -1.299100      25.46
 O      -4.756354    -0.804614     0.492595     179.87
 H      -4.231743    -0.150527     1.116750      21.25
 C      -2.628678    -1.739140    -0.239618      94.32
 H      -2.149365    -1.779103    -1.173088      26.01
 C      -2.718610    -3.035825     0.556661     122.23
 O      -3.529967    -3.950485    -0.231940     221.92
 H      -3.300032    -4.167007    -1.088859      31.25
 H      -2.985198    -2.945357     1.552288      25.95
 H      -1.715021    -3.493116     1.028840      24.70
 C       1.739419    -0.968430    -0.644550      38.25
 H       2.356075    -1.851863    -1.071631      19.31
 C       1.293858     1.075398     0.745948      63.15
 H       1.585115     1.780420     1.357603      24.20
 C      -0.018561     0.607651     0.893081      -2.93
 O      -0.858122     1.375924     1.621525     209.86
 C      -0.871102     2.813347     1.367260     108.76
 H      -0.773446     3.253393     2.277560      26.37
 H      -0.193484     3.104323     0.458308      23.14
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 H      -1.865838     2.985407     1.235815      25.68
 C      -0.569747    -0.630398     0.314812      -7.79
 O      -1.942534    -0.727926     0.526423     135.51
 C       0.388435    -1.373101    -0.540629      66.32
 H       0.155823    -2.332404    -0.765298      21.90
 C       2.187571     0.273858    -0.090417      18.12
 C       3.756246     0.436740    -0.337318      92.18
 H       3.993610     0.048776    -1.291756      26.24
 O       3.974873     1.882491    -0.457274     216.03
 H       4.446157     2.425696     0.298586      18.56
 C       4.775123    -0.324420     0.476853      76.04
 H       4.552814    -0.237169     1.737835      21.70
 O       4.634165    -1.832596     0.545331     272.38
 H       4.726798    -2.141570    -0.381469      28.72
 C       6.143815     0.196437     0.182434     100.83
 O       6.727647     1.621153     0.033714     219.19
 H       6.815637     2.173281     0.881970      25.96
 H       6.657107    -0.382310    -0.688284      27.67
 H       7.024250    -0.445989     0.783541      27.03
55
name= lig-ACN-Water-frame_569
 C      -3.267632    -0.066899    -2.892336      42.50
 H      -2.929840    -0.980128    -3.205844      19.92
 C      -4.055463     1.617446    -1.115713      63.79
 H      -4.399290     1.696730    -0.174968      23.76
 C      -3.904216     2.666973    -2.077957      14.39
 O      -4.102864     4.013862    -1.895932     216.04
 C      -4.834710     4.682648    -0.814205     129.78
 H      -5.941946     4.426365    -0.758613      26.90
 H      -5.039663     5.659205    -1.202735      27.38
 H      -4.417317     4.900624     0.192636      27.77
 C      -3.303636     2.400747    -3.436277      14.16
 O      -3.179672     3.464022    -4.282770     194.06
 H      -3.176361     4.362775    -3.859652      23.76
 C      -3.025517     1.065603    -3.711428      64.25
 H      -2.735691     0.730376    -4.719771      31.93
 C      -3.733474     0.214052    -1.474824      19.72
 C      -3.943561    -1.015867    -0.764465      92.65
 H      -4.675935    -1.737091    -1.254660      24.73
 O      -4.749326    -0.715900     0.475093     161.75
 H      -4.219956    -0.319728     1.180877      27.53
 C      -2.637154    -1.779493    -0.361568      80.10
 H      -2.027430    -2.141711    -1.106573      26.22
 C      -2.669543    -2.980445     0.584947     107.03
 O      -3.548947    -3.976074    -0.243389     192.19
 H      -2.792322    -4.153494    -0.789070      31.41
 H      -3.292982    -2.806745     1.467496      25.03
 H      -1.637128    -3.361005     0.273317      22.31
 C       1.715257    -1.045354    -0.626098      38.30
 H       2.573611    -1.558388    -1.194534      19.44
 C       1.376482     0.962279     0.658387      64.08
 H       1.695457     1.780952     0.981385      24.40
 C      -0.029073     0.592046     0.875034     -15.12
 O      -0.909777     1.380914     1.695113     193.59
 C      -0.955275     2.849667     1.376204     114.72
 H      -0.534724     3.326527     2.129844      26.61
 H      -0.217089     3.190128     0.585545      24.94
 H      -1.912328     3.109670     0.956250      24.83
 C      -0.498271    -0.609204     0.377737      -7.34
 O      -1.904562    -0.733007     0.549734     105.11
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 C       0.333464    -1.451749    -0.511162      79.88
 H       0.040488    -2.293746    -1.089869      21.30
 C       2.206146     0.159693    -0.102703      28.21
 C       3.681872     0.454594    -0.359446      89.59
 H       3.799926     0.165913    -1.393479      24.46
 O       3.983316     1.914874    -0.411906     259.07
 H       4.163815     2.150049     0.579371      22.09
 C       4.749242    -0.244064     0.622354      63.19
 H       4.514415     0.284589     1.742693      22.47
 O       4.623887    -1.679199     0.525766     302.07
 H       4.797974    -1.897123    -0.373133      31.54
 C       6.247953     0.191073     0.168155      83.26
 O       6.629559     1.534183     0.057362     241.10
 H       6.915595     1.880638     0.931048      29.84
 H       6.260304    -0.223335    -0.962259      27.53
 H       6.654000    -0.168336     1.254878      25.74
55
name= lig-ACN-Water-frame_570
 C      -3.199218    -0.021065    -2.807188      65.92
 H      -3.157142    -1.058811    -3.112894      25.98
 C      -4.019071     1.537931    -1.108805      68.09
 H      -4.438192     1.808898    -0.236651      21.90
 C      -3.826962     2.598266    -2.100691      -5.17
 O      -4.100639     4.091583    -1.990904     161.37
 C      -4.858709     4.731957    -0.789786     104.22
 H      -5.819211     4.171358    -0.757369      26.74
 H      -4.676561     5.757421    -1.093243      26.07
 H      -4.316738     4.520071     0.204992      25.62
 C      -3.295022     2.395288    -3.342112      21.35
 O      -3.155485     3.489570    -4.304197     202.95
 H      -3.101654     4.391804    -3.796496      24.00
 C      -3.026459     0.999578    -3.786336      58.04
 H      -2.608639     0.977063    -4.841287      17.10
 C      -3.580632     0.255737    -1.554477      33.05
 C      -3.963093    -1.030162    -0.649380      81.26
 H      -4.422163    -1.800670    -1.403080      24.55
 O      -4.764269    -0.678268     0.460293     230.32
 H      -4.223044    -0.178033     1.057479      26.79
 C      -2.580265    -1.676607    -0.358930      87.32
 H      -2.206926    -1.660803    -1.335172      23.84
 C      -2.746811    -3.022347     0.411300     120.29
 O      -3.499669    -4.013877    -0.194908     208.93
 H      -3.162121    -4.593004    -1.065922      25.90
 H      -3.182284    -2.783971     1.458379      23.93
 H      -1.873088    -3.354052     1.122270      24.58
 C       1.642390    -1.153000    -0.670399      53.60
 H       1.992270    -1.779231    -1.522861      20.91
 C       1.354460     0.920624     0.642520      63.96
 H       1.709702     1.780362     0.857432      22.14
 C       0.065920     0.621021     0.928387       1.32
 O      -0.930545     1.410551     1.717099     190.30
 C      -0.969497     2.856082     1.368741     116.70
 H      -0.800463     3.449229     2.181550      26.28
 H      -0.370351     2.898675     0.510438      24.94
 H      -2.041805     3.162121     1.210052      24.28
 C      -0.503330    -0.602271     0.306237      -2.24
 O      -1.827427    -0.821592     0.489516     183.15
 C       0.329684    -1.466945    -0.385912      54.84
 H      -0.285801    -2.126029    -1.056868      20.16
 C       2.262218    -0.005579    -0.081137      31.95
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 C       3.637848     0.537258    -0.397668     101.41
 H       4.042549     0.096415    -1.322450      24.03
 O       3.944519     1.878629    -0.401326     273.31
 H       4.204932     2.237014     0.499429      22.79
 C       4.623421    -0.077560     0.614678      99.98
 H       4.459339     0.023560     1.793317      23.58
 O       4.636709    -1.495357     0.531577     256.66
 H       4.792035    -1.791336    -0.408028      28.82
 C       6.312675     0.097779     0.274841      75.16
 O       6.544126     1.491562     0.038694     206.64
 H       7.086213     1.973005     0.712470      29.23
 H       6.560783    -0.536594    -0.774514      29.65
 H       7.285729    -0.581172     0.641188      27.80
55
name= lig-ACN-Water-frame_571
 C      -3.099067     0.064284    -2.897944      66.66
 H      -2.971702    -1.019739    -3.303076      25.07
 C      -3.944982     1.596085    -1.196556      71.78
 H      -4.403473     1.665791    -0.236228      22.85
 C      -3.784427     2.713679    -2.033060      32.91
 O      -4.115242     4.052687    -1.979389     277.85
 C      -4.779626     4.655441    -0.862939     123.50
 H      -5.874956     4.492299    -0.790157      29.84
 H      -4.832619     5.698475    -0.652404      26.76
 H      -4.251791     4.199435     0.034827      25.84
 C      -3.267306     2.372488    -3.422896      22.44
 O      -3.109449     3.393018    -4.279493     156.22
 H      -3.286805     4.251651    -3.805125      24.00
 C      -2.998028     1.117383    -3.825966      -3.12
 H      -2.748435     0.722801    -4.867599      16.61
 C      -3.641356     0.258330    -1.517853      37.33
 C      -3.876404    -0.919256    -0.612070      90.40
 H      -4.643332    -1.698498    -1.115933      21.39
 O      -4.808666    -0.669571     0.465325     151.06
 H      -4.446612    -0.122643     1.254057      21.80
 C      -2.554922    -1.678670    -0.361205      90.13
 H      -2.001244    -1.881202    -1.276757      20.94
 C      -2.776015    -3.009174     0.399954     105.98
 O      -3.523736    -4.155551    -0.181254     201.63
 H      -3.164170    -4.150310    -1.157587      29.36
 H      -3.657249    -2.663217     0.976826      22.33
 H      -1.745403    -3.433830     0.655149      23.64
 C       1.639497    -1.227165    -0.749935      37.34
 H       2.265035    -1.842925    -1.394267      18.39
 C       1.425755     0.881866     0.663966      44.92
 H       1.867900     1.675866     1.172955      20.79
 C      -0.031745     0.585303     0.998602      14.54
 O      -0.856688     1.401762     1.680663     230.23
 C      -0.992879     2.842137     1.359364     110.98
 H      -0.543484     3.257305     2.160758      25.63
 H      -0.547680     3.286069     0.553324      25.44
 H      -2.141066     2.875844     1.170910      21.71
 C      -0.492773    -0.526659     0.358656      18.53
 O      -1.809718    -0.841595     0.512561     223.62
 C       0.263161    -1.469263    -0.371062      51.95
 H      -0.089274    -2.544118    -0.700305      18.89
 C       2.180628    -0.022125    -0.119600      11.63
 C       3.767518     0.439123    -0.402672      65.15
 H       3.855578     0.166560    -1.497078      23.22
 O       3.847391     1.963188    -0.455436     202.84
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 H       4.399580     2.224823     0.268104      24.87
 C       4.825498    -0.110986     0.612331     104.03
 H       4.403531     0.387538     1.532722      24.71
 O       4.579278    -1.499018     0.559769     277.39
 H       4.598465    -1.771892    -0.477910      25.64
 C       6.234123     0.074174     0.282996      81.99
 O       6.591187     1.511301    -0.017605     219.40
 H       6.784298     1.933279     0.881640      27.43
 H       6.168239    -0.352222    -0.855352      28.66
 H       6.707409    -0.332630     1.322114      27.11
55
name= lig-ACN-Water-frame_572
 C      -3.103736     0.067536    -2.899556      75.25
 H      -2.587552    -0.974354    -3.218263      19.12
 C      -3.936889     1.689400    -1.177132      65.57
 H      -4.407411     1.945022    -0.160512      20.78
 C      -3.707217     2.709097    -2.148339      11.02
 O      -4.119264     4.060455    -1.999480     231.55
 C      -4.740602     4.505719    -0.778862     128.52
 H      -5.791112     4.300122    -0.985364      27.26
 H      -4.332761     5.400091    -1.058848      25.62
 H      -4.492178     4.103126     0.244280      26.61
 C      -3.282260     2.437139    -3.370261      23.07
 O      -3.051063     3.410739    -4.343503     203.68
 H      -3.347734     4.265014    -4.045287      23.10
 C      -2.949942     1.106739    -3.807035      83.21
 H      -2.748938     1.143969    -4.910554      26.24
 C      -3.639896     0.348253    -1.666089      38.46
 C      -3.878810    -0.868070    -0.718092      66.28
 H      -4.410814    -1.651049    -1.491637      24.43
 O      -4.826811    -0.634302     0.528290     108.08
 H      -4.145603    -0.378760     1.332223      21.56
 C      -2.601813    -1.741379    -0.383236      59.42
 H      -1.980883    -1.899482    -1.318522      23.36
 C      -2.895747    -3.016447     0.494513     105.21
 O      -3.533143    -4.247687    -0.286546     184.15
 H      -3.387962    -4.135109    -1.176146      32.86
 H      -3.034564    -2.928742     1.595333      24.13
 H      -1.843353    -3.320746     0.839216      24.84
 C       1.643134    -1.125802    -0.684896      52.10
 H       2.265601    -1.873673    -1.080280      23.35
 C       1.419493     0.772142     0.773484      62.35
 H       1.978833     1.617562     1.270072      21.67
 C       0.124061     0.598856     0.897364      -0.72
 O      -0.793781     1.404963     1.672207     185.13
 C      -1.007103     2.822970     1.382979     116.70
 H      -0.720267     3.511459     2.128469      26.08
 H      -0.559190     2.912948     0.489514      28.15
 H      -2.155281     3.168142     1.404608      23.53
 C      -0.497569    -0.648058     0.357134     -29.85
 O      -1.869328    -0.809830     0.639806      90.40
 C       0.336284    -1.510145    -0.431536      63.25
 H      -0.173301    -2.567482    -0.487711      20.89
 C       2.241479     0.044950    -0.209712      20.59
 C       3.710237     0.455858    -0.458103      87.84
 H       4.201625     0.021669    -1.429432      24.79
 O       3.791835     1.944718    -0.556234     204.30
 H       4.127821     2.306826     0.366044      21.83
 C       4.707520    -0.130435     0.553610      97.76
 H       4.711500     0.079670     1.574782      25.90
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 O       4.519252    -1.650376     0.629896     223.84
 H       4.629363    -2.024903    -0.358047      27.36
 C       6.230973     0.223202     0.198366     103.17
 O       6.678988     1.499294    -0.031001     261.72
 H       6.833237     2.079205     0.777826      25.79
 H       6.947362    -0.589169    -0.398545      27.51
 H       6.923122    -0.186253     1.094383      27.54
55
name= lig-ACN-Water-frame_573
 C      -3.086573     0.093080    -2.922541      47.66
 H      -2.902238    -1.101539    -3.075767      25.62
 C      -3.929181     1.699235    -1.239059      77.55
 H      -4.378103     1.874045    -0.130117      19.53
 C      -3.757060     2.734810    -2.139811      28.46
 O      -4.053314     3.998258    -2.011942     224.26
 C      -4.756965     4.474603    -0.727419     117.49
 H      -5.841615     4.430418    -0.666433      28.84
 H      -4.702529     5.412997    -0.245285      26.91
 H      -4.288803     3.847035     0.037423      26.79
 C      -3.191297     2.463233    -3.507717      25.93
 O      -3.019336     3.490786    -4.456099     205.14
 H      -3.083508     4.373950    -3.948156      25.97
 C      -2.892768     1.155206    -3.843531      47.62
 H      -2.352618     0.894569    -4.728506      19.23
 C      -3.627073     0.402062    -1.606820      43.56
 C      -3.978673    -0.887301    -0.769824      91.30
 H      -4.829748    -1.580625    -1.353374      25.08
 O      -4.705751    -0.623231     0.446889     151.86
 H      -4.096248    -0.382039     1.206528      24.52
 C      -2.772197    -1.679162    -0.185950      75.28
 H      -2.072343    -1.948232    -1.072515      22.53
 C      -2.873829    -3.163815     0.504536     105.67
 O      -3.542932    -4.196432    -0.301061     197.95
 H      -3.307839    -3.939226    -1.269844      29.63
 H      -3.720533    -3.055846     1.204108      23.32
 H      -1.871686    -3.587846     0.553015      24.46
 C       1.702253    -1.112427    -0.654279      43.46
 H       2.237385    -1.669057    -1.382513      23.01
 C       1.595059     0.792054     0.774430      -8.69
 H       1.838147     1.780979     1.416548      17.52
 C       0.044791     0.532341     0.825081     -53.69
 O      -0.736040     1.354806     1.712764     150.52
 C      -0.961263     2.815400     1.367264     104.54
 H      -0.382880     3.336104     2.034017      24.69
 H      -0.719245     3.154171     0.400759      26.49
 H      -2.156529     2.750917     1.314450      21.86
 C      -0.526573    -0.668225     0.361806      15.76
 O      -1.863642    -0.852902     0.670824     116.27
 C       0.339522    -1.525556    -0.360827      60.88
 H       0.192805    -2.400854    -1.056912      21.60
 C       2.263566     0.110140    -0.181565      32.15
 C       3.645649     0.481437    -0.516720      83.73
 H       3.785819     0.074950    -1.647173      24.68
 O       3.781640     1.876499    -0.634798     224.83
 H       3.919590     2.278077     0.354127      24.24
 C       4.610132    -0.275894     0.535563      72.08
 H       4.203445     0.116443     1.382161      29.77
 O       4.505272    -1.713166     0.653716     278.14
 H       4.765412    -2.081702    -0.187022      31.52
 C       6.431824     0.159067     0.252579      72.16
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 O       6.758813     1.588307    -0.103510     158.16
 H       6.993943     2.006951     0.750154      27.20
 H       6.456243    -0.364634    -0.863820      27.42
 H       6.701987    -0.116473     1.313960      26.86
55
name= lig-ACN-Water-frame_574
 C      -3.108637     0.150638    -2.890836      44.01
 H      -3.036892    -0.871118    -3.473861      19.95
 C      -3.931355     1.640120    -1.275585      36.42
 H      -4.487184     1.886259    -0.215987      19.83
 C      -3.750265     2.706743    -2.296075     -11.09
 O      -4.088315     4.189769    -1.917369     176.10
 C      -4.732730     4.359307    -0.648109     118.66
 H      -5.719744     4.036007    -0.876357      26.63
 H      -4.376452     5.408996    -0.581740      25.46
 H      -4.370024     3.706559     0.134775      26.05
 C      -3.131483     2.508046    -3.588658      13.29
 O      -3.014254     3.564100    -4.478734     237.23
 H      -2.828721     4.476587    -4.023589      25.44
 C      -2.760954     1.131023    -3.880911      40.17
 H      -2.403691     0.862225    -4.823454      27.46
 C      -3.610931     0.261689    -1.572439      23.01
 C      -3.986681    -0.894595    -0.676764      92.97
 H      -4.589930    -1.718346    -1.401263      22.98
 O      -4.722775    -0.538443     0.445721     177.55
 H      -4.132417    -0.069044     1.011766      26.56
 C      -2.726913    -1.795732    -0.182748      73.52
 H      -2.176536    -1.943016    -1.203505      22.06
 C      -2.960914    -3.193060     0.498713     118.74
 O      -3.585703    -4.112778    -0.398249     225.04
 H      -3.152728    -4.166167    -1.436721      22.70
 H      -3.424499    -3.168414     1.517194      24.01
 H      -2.065712    -3.373291     1.049069      25.45
 C       1.694930    -1.096455    -0.689737      52.97
 H       2.197953    -1.540429    -1.538626      21.88
 C       1.360294     0.878127     0.750445      51.73
 H       2.032749     1.803202     1.258840      18.70
 C       0.116580     0.543012     0.945541      36.82
 O      -0.653931     1.306381     1.692481     240.82
 C      -0.911508     2.695024     1.338383     112.56
 H      -0.446248     3.358919     2.014079      26.91
 H      -0.648659     2.867055     0.307526      26.79
 H      -1.986676     3.047679     1.699429      24.49
 C      -0.486115    -0.645734     0.350946     -35.52
 O      -1.915610    -0.920779     0.691139     110.67
 C       0.388847    -1.521619    -0.390106      64.31
 H      -0.216166    -2.231695    -0.888763      22.72
 C       2.240932     0.038536    -0.100238      12.58
 C       3.679355     0.358296    -0.631342      75.85
 H       3.808440     0.066318    -1.807213      21.30
 O       3.821196     1.873982    -0.661286     234.79
 H       4.186217     2.249723     0.179792      23.70
 C       4.683807    -0.262335     0.497999      92.41
 H       4.461961     0.080999     1.388882      27.01
 O       4.537410    -1.707052     0.612552     286.08
 H       4.625803    -2.073763    -0.255092      30.01
 C       6.314101     0.167939     0.290161      87.30
 O       6.792950     1.544588    -0.101352     223.54
 H       6.812399     2.241510     0.603986      27.19
 H       6.707055    -0.564281    -0.682763      27.62
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 H       7.100752    -0.361505     0.911642      28.74
55
name= lig-ACN-Water-frame_575
 C      -3.069870     0.074556    -3.000777      40.31
 H      -2.829669    -1.011516    -3.226744      20.30
 C      -3.930195     1.655749    -1.427502      65.97
 H      -4.447757     1.986611    -0.429084      22.17
 C      -3.747588     2.758858    -2.286218      15.65
 O      -4.033936     4.139283    -1.925047     209.97
 C      -4.720553     4.268148    -0.606443     130.57
 H      -5.783961     4.149795    -0.478717      27.38
 H      -4.835298     5.355045    -0.245015      25.79
 H      -4.207735     3.910550     0.237504      28.41
 C      -3.128021     2.557419    -3.526476       7.11
 O      -2.972838     3.612809    -4.488512     201.17
 H      -3.103569     4.434321    -3.942011      24.19
 C      -2.740744     1.201026    -3.839839      64.97
 H      -2.559498     1.005031    -4.852821      29.87
 C      -3.609291     0.304182    -1.659785       3.47
 C      -3.846543    -1.007698    -0.635480      55.37
 H      -4.704201    -1.736603    -1.181835      22.20
 O      -4.832778    -0.394630     0.539675      39.18
 H      -4.212612     0.029964     1.247773      24.79
 C      -2.637632    -1.854509    -0.271185      71.65
 H      -1.975721    -2.184772    -1.164683      21.17
 C      -2.993463    -3.111681     0.552691     114.02
 O      -3.667046    -4.073872    -0.444450     134.11
 H      -3.072486    -3.930395    -1.373731      25.48
 H      -3.813717    -2.914228     1.226091      24.86
 H      -2.172324    -3.678733     0.646565      25.73
 C       1.611440    -1.116660    -0.768067      37.60
 H       2.268587    -1.839733    -1.318979      19.81
 C       1.471306     0.873278     0.603992      23.25
 H       1.668234     2.014227     1.137527      21.11
 C       0.087193     0.460266     1.009850      -1.62
 O      -0.738792     1.313953     1.807393     216.06
 C      -0.842394     2.658209     1.377227     117.66
 H      -0.133917     3.225717     1.702574      28.88
 H      -0.719087     2.690769     0.226485      26.95
 H      -1.974503     2.807681     1.442097      25.13
 C      -0.496713    -0.678633     0.418941      16.56
 O      -1.823382    -0.979254     0.672851     126.08
 C       0.267274    -1.478541    -0.469351      64.09
 H       0.063707    -2.420126    -0.741096      24.57
 C       2.254310     0.009277    -0.126615      24.27
 C       3.704787     0.395725    -0.503325      89.78
 H       4.021802    -0.201164    -1.486626      25.51
 O       3.883514     1.831376    -0.688309     197.19
 H       4.329608     2.041380     0.126145      28.06
 C       4.824988    -0.165914     0.436797     110.14
 H       4.569149     0.157366     1.312863      30.81
 O       4.620315    -1.650875     0.523621     244.56
 H       4.582848    -1.985784    -0.464509      26.70
 C       6.249566     0.120866     0.181407      99.93
 O       6.727847     1.425154    -0.059695     232.74
 H       6.631283     1.956429     0.792734      26.56
 H       6.561984    -0.452572    -0.870241      27.49
 H       6.596684    -0.160670     1.244364      28.28
55
name= lig-ACN-Water-frame_576
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 C      -2.973600     0.041630    -3.046398      53.25
 H      -2.545235    -0.859118    -3.452412      23.97
 C      -3.986077     1.662113    -1.451147      65.92
 H      -4.368092     1.683847    -0.432661      22.10
 C      -3.708059     2.798061    -2.220873      33.96
 O      -4.043046     4.024943    -1.867604     212.31
 C      -4.724041     4.290842    -0.535921      88.97
 H      -5.418574     3.554578    -0.640878      27.24
 H      -4.708133     5.485193    -0.532109      23.18
 H      -3.998346     3.840653     0.069425      29.00
 C      -3.117012     2.591509    -3.534241      17.53
 O      -2.929953     3.595391    -4.419337     192.74
 H      -3.154666     4.498767    -4.207359      24.61
 C      -2.839224     1.247523    -3.867682      75.00
 H      -2.266072     1.135626    -4.782912      23.19
 C      -3.592362     0.299065    -1.785605      14.91
 C      -3.900441    -0.833495    -0.650396      53.49
 H      -4.652914    -1.718535    -1.096983      24.43
 O      -4.755764    -0.323105     0.538735      98.04
 H      -4.201205    -0.393145     1.460622      21.98
 C      -2.557669    -1.779131    -0.199496      82.29
 H      -2.024254    -1.968686    -1.190752      24.09
 C      -3.040622    -3.146039     0.430782     128.84
 O      -3.784054    -4.001435    -0.380396     254.90
 H      -3.644945    -3.911955    -1.380616      27.12
 H      -3.648958    -2.803562     1.250467      27.40
 H      -2.369737    -3.413788     1.126877      29.41
 C       1.619557    -1.145625    -0.758804      40.97
 H       2.158412    -1.981334    -1.339760      20.73
 C       1.412080     0.804812     0.594922      43.48
 H       2.045828     1.853693     0.821599      21.05
 C       0.117172     0.466405     0.999469      -3.62
 O      -0.771906     1.211116     1.933490     185.32
 C      -0.827666     2.669616     1.308404      94.78
 H      -0.137882     3.216442     1.736947      26.69
 H      -0.769528     2.586699     0.131948      25.36
 H      -1.668638     3.231434     1.727747      25.78
 C      -0.446336    -0.723069     0.421882       2.24
 O      -1.778858    -1.054925     0.673129     159.63
 C       0.242299    -1.476231    -0.521211      66.60
 H      -0.182091    -2.331398    -0.904163      21.80
 C       2.245886     0.022749    -0.262836      17.41
 C       3.736432     0.400945    -0.456914      99.83
 H       3.853772     0.106312    -1.576893      24.10
 O       3.953403     1.802835    -0.693165     190.31
 H       4.110505     2.468891     0.100745      26.04
 C       4.728692    -0.158792     0.479961     117.04
 H       4.630102     0.171100     1.380626      31.05
 O       4.719091    -1.550774     0.419720     262.15
 H       4.891933    -1.876830    -0.599174      26.39
 C       6.299238     0.000603     0.109443      88.90
 O       6.642851     1.407088    -0.023969     213.15
 H       6.999443     1.779418     0.837176      24.93
 H       6.676693    -0.751644    -0.791630      30.59
 H       6.921744    -0.615984     0.912220      29.67
55
name= lig-ACN-Water-frame_577
 C      -2.910111     0.172304    -3.090647      65.38
 H      -2.600221    -0.784581    -3.416083      28.35
 C      -4.000100     1.536755    -1.384132      70.17
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 H      -4.449997     1.753728    -0.509568      21.72
 C      -3.684334     2.680776    -2.193455      15.05
 O      -4.067671     4.086609    -1.816568     240.92
 C      -4.605932     4.180571    -0.549363     153.73
 H      -5.543723     3.875342    -0.244325      28.22
 H      -5.205596     5.252452    -0.571584      25.86
 H      -4.140991     4.308928     0.381770      27.62
 C      -3.170842     2.562739    -3.463051      18.67
 O      -2.870110     3.593552    -4.407221     210.87
 H      -2.918998     4.384623    -3.820892      24.85
 C      -2.824991     1.231356    -3.964758      40.09
 H      -2.342964     1.177715    -5.002346      18.35
 C      -3.608960     0.282032    -1.764450      38.98
 C      -3.916908    -0.698221    -0.674539      95.14
 H      -4.618873    -1.498485    -1.323398      24.97
 O      -4.585703    -0.299150     0.462046     206.06
 H      -3.881393    -0.236475     1.244429      21.40
 C      -2.680429    -1.667255    -0.271902      76.68
 H      -2.152167    -1.783743    -1.227793      24.17
 C      -3.091308    -3.016843     0.462969     116.11
 O      -3.941762    -3.973323    -0.339838     222.90
 H      -3.512094    -4.001818    -1.132691      34.41
 H      -3.795553    -2.791053     1.206038      25.56
 H      -2.296519    -3.605264     0.578721      27.23
 C       1.679098    -1.230849    -0.812998      49.62
 H       2.326173    -1.666300    -1.657861      16.30
 C       1.384620     0.801277     0.628496      44.10
 H       1.783556     1.735528     1.256318      20.39
 C       0.082649     0.442499     1.023792      11.25
 O      -0.698088     1.193585     1.870470     235.23
 C      -0.802900     2.610958     1.394502     106.73
 H       0.052484     2.991277     1.452005      27.31
 H      -0.959204     2.608531     0.159476      23.41
 H      -1.695209     2.957423     1.753864      25.75
 C      -0.432079    -0.702796     0.393740      -2.31
 O      -1.752779    -1.073831     0.792895     177.29
 C       0.361156    -1.517534    -0.550167      58.65
 H      -0.268449    -2.167932    -1.194498      20.69
 C       2.166300     0.019199    -0.296961      19.19
 C       3.681003     0.450555    -0.630185      60.22
 H       4.124928    -0.069330    -1.466614      26.79
 O       3.966163     1.918250    -0.703082     185.87
 H       3.990585     1.999492     0.309923      25.81
 C       4.855725    -0.224892     0.528039      84.37
 H       4.586607    -0.017560     1.444334      30.65
 O       4.726571    -1.650592     0.381064     265.25
 H       4.739015    -1.848534    -0.698408      25.81
 C       6.313221    -0.016787     0.114834      96.56
 O       6.653608     1.387150    -0.007502     226.07
 H       7.039125     1.724742     0.824093      29.16
 H       6.233198    -0.225436    -1.097762      30.17
 H       7.075258    -0.522135     0.767846      30.66
55
name= lig-ACN-Water-frame_578
 C      -2.967564     0.169752    -3.038615      59.33
 H      -2.684572    -0.846485    -3.298595      21.20
 C      -3.991919     1.645847    -1.344770      85.30
 H      -4.486747     1.626047    -0.482923      22.38
 C      -3.760231     2.717493    -2.163272       9.98
 O      -4.024415     3.965819    -1.812455     213.87
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 C      -4.697442     4.276721    -0.423067      83.58
 H      -5.097719     3.363989    -0.333832      27.69
 H      -5.097062     5.410612    -0.617072      23.05
 H      -3.735287     4.209060     0.037121      26.54
 C      -3.143482     2.517190    -3.555490       0.21
 O      -2.835072     3.583725    -4.300476     107.53
 H      -2.906711     4.572509    -4.052623      17.47
 C      -2.784790     1.279654    -3.973602      69.32
 H      -2.638429     1.059199    -5.116713      24.52
 C      -3.530032     0.348765    -1.774038      24.74
 C      -3.838885    -0.820362    -0.799680      89.20
 H      -4.744836    -1.582260    -1.085525      23.15
 O      -4.469234    -0.228274     0.438791     141.10
 H      -3.876919     0.147626     1.093040      24.53
 C      -2.774370    -1.648621    -0.319144      88.24
 H      -2.138891    -1.990357    -1.066901      24.58
 C      -3.182861    -2.916816     0.431273     120.77
 O      -4.052393    -3.890027    -0.307720     213.01
 H      -3.635834    -4.235734    -1.174163      28.47
 H      -3.269852    -2.824937     1.448517      27.95
 H      -2.243436    -3.245436     0.534382      27.99
 C       1.737516    -1.118073    -0.916807     105.73
 H       2.199120    -1.740742    -1.745668      14.92
 C       1.457215     0.776860     0.667704      47.74
 H       1.919510     1.647453     1.180432      19.26
 C       0.112423     0.350617     0.956629       6.07
 O      -0.639151     1.206059     1.802867     246.94
 C      -0.786166     2.518839     1.441299     125.48
 H      -0.122753     3.173698     1.595598      28.55
 H      -1.296680     2.595315     0.303265      22.49
 H      -1.395694     2.937533     2.130702      27.76
 C      -0.495905    -0.775579     0.355654       9.48
 O      -1.747219    -1.077542     0.817324     143.70
 C       0.360959    -1.541437    -0.556326      78.58
 H       0.040998    -2.497008    -1.151914      16.29
 C       2.271912     0.079356    -0.256831      41.24
 C       3.719312     0.469205    -0.633797      74.54
 H       3.750323     0.322367    -1.680863      25.32
 O       3.884952     1.967491    -0.649840     241.94
 H       4.253979     2.391459     0.077745      28.16
 C       4.831706    -0.336699     0.460345      76.72
 H       4.674405    -0.038215     1.419628      26.40
 O       4.678771    -1.826856     0.401322     239.86
 H       4.574412    -2.050082    -0.636255      23.29
 C       6.275264     0.099568     0.023135      98.72
 O       6.761526     1.428926     0.016293     279.43
 H       6.591087     1.904949     0.870573      29.52
 H       6.435344    -0.439274    -1.064782      28.86
 H       6.890202    -0.668038     0.567834      30.17
55
name= lig-ACN-Water-frame_579
 C      -3.015679     0.123205    -3.047548      59.81
 H      -2.746014    -0.898886    -3.452506      23.80
 C      -3.944473     1.636125    -1.355349      67.36
 H      -4.348728     1.863861    -0.381976      19.64
 C      -3.763181     2.711082    -2.264489      26.29
 O      -4.058242     4.041077    -1.815929     237.91
 C      -4.582394     4.255635    -0.441409     130.85
 H      -5.424728     3.747885     0.001510      26.45
 H      -5.319421     5.208570    -0.469635      26.67
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 H      -3.931769     4.522095     0.455025      26.61
 C      -3.141020     2.562808    -3.456847      19.26
 O      -2.794099     3.626320    -4.303450     271.03
 H      -3.030504     4.349833    -3.660495      25.37
 C      -2.832762     1.181294    -3.900409      53.19
 H      -2.327770     1.052218    -4.961840      21.10
 C      -3.510303     0.392028    -1.754023      38.97
 C      -3.871209    -0.730023    -0.788015      77.47
 H      -4.557923    -1.456633    -1.450209      25.35
 O      -4.458153    -0.168925     0.394242     185.22
 H      -3.734354    -0.257105     1.024347      25.19
 C      -2.626267    -1.767404    -0.304044     101.04
 H      -2.119714    -1.987773    -1.176092      26.06
 C      -3.117192    -3.017860     0.429354     121.37
 O      -4.090503    -3.749635    -0.225167     124.59
 H      -3.707479    -3.970837    -1.261622      26.57
 H      -3.817793    -2.703416     1.136704      26.06
 H      -2.384935    -3.700500     0.661665      27.85
 C       1.638260    -0.937006    -0.922730      52.88
 H       2.285895    -1.502881    -1.569069      21.90
 C       1.549644     0.696411     0.685686      62.30
 H       1.849499     1.575192     1.092069      22.27
 C       0.217531     0.362299     0.867024       3.04
 O      -0.575132     1.078830     1.802184     175.20
 C      -0.840094     2.609723     1.500906     101.96
 H       0.016603     2.932352     1.333603      26.92
 H      -1.438400     2.829347     0.427969      22.56
 H      -1.480797     2.820813     2.236488      26.08
 C      -0.418292    -0.816565     0.329367      -9.40
 O      -1.839797    -1.109628     0.679376     189.71
 C       0.405518    -1.472629    -0.577555      67.32
 H      -0.160231    -2.379516    -1.009822      17.81
 C       2.365224     0.039562    -0.270391      39.99
 C       3.746042     0.506576    -0.520434     105.54
 H       4.053106     0.156974    -1.441538      25.30
 O       3.806142     1.990331    -0.571781     216.68
 H       4.317751     2.232237     0.260335      23.60
 C       4.713081    -0.371975     0.241447      99.82
 H       4.554466    -0.086872     1.241828      25.64
 O       4.628363    -1.861889     0.419959     270.95
 H       4.695775    -2.179583    -0.532568      26.88
 C       6.282006    -0.031588    -0.077700      79.92
 O       6.842641     1.513279     0.029222     204.87
 H       6.554244     2.076806     0.822982      27.15
 H       6.591744    -0.097534    -1.170182      27.38
 H       6.905009    -0.401245     0.726472      28.34
55
name= lig-ACN-Water-frame_580
 C      -3.064776     0.073194    -3.038766      49.51
 H      -2.839130    -1.027655    -3.356831      23.25
 C      -3.866077     1.674720    -1.399338      62.24
 H      -4.210234     1.826299    -0.281045      18.50
 C      -3.773666     2.772807    -2.196006      14.57
 O      -4.123086     4.138960    -1.799686     201.56
 C      -4.586566     4.328107    -0.453258     107.75
 H      -5.230410     3.425869    -0.291579      24.68
 H      -4.937514     5.416094    -0.672611      23.40
 H      -3.594548     4.361300     0.202400      24.51
 C      -3.088303     2.530148    -3.506197      14.74
 O      -2.776342     3.598761    -4.298130     206.02
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 H      -2.682788     4.514183    -4.041898      24.23
 C      -2.845474     1.225939    -3.878144      63.57
 H      -2.220651     1.106261    -4.824910      24.21
 C      -3.516317     0.306069    -1.712846      20.24
 C      -3.786861    -0.773648    -0.725949      88.37
 H      -4.709808    -1.376601    -1.156092      24.07
 O      -4.489509    -0.190162     0.373555     182.75
 H      -4.151712    -0.148570     1.341062      20.93
 C      -2.556439    -1.803117    -0.415063      80.17
 H      -2.019672    -2.117282    -1.272067      25.55
 C      -3.093447    -3.091268     0.548479     109.58
 O      -4.151823    -3.718719    -0.314613     180.17
 H      -3.824833    -3.766470    -1.290457      28.51
 H      -3.333906    -2.558622     1.441155      27.40
 H      -2.376902    -3.660472     1.045385      28.09
 C       1.692287    -0.989628    -1.017830      41.95
 H       2.039518    -1.421391    -1.916878      21.35
 C       1.598196     0.734229     0.743718      68.48
 H       1.973382     1.397674     1.338076      24.60
 C       0.173811     0.390212     0.925116     -18.91
 O      -0.570162     1.070894     1.806459     208.07
 C      -0.837480     2.540773     1.548992     112.44
 H      -0.079381     3.165121     1.474871      26.86
 H      -1.590508     2.517803     0.615107      23.21
 H      -1.182848     3.007025     2.412292      27.20
 C      -0.425037    -0.745122     0.339917      22.68
 O      -1.712506    -1.060060     0.521584     181.78
 C       0.348766    -1.431726    -0.642872      67.28
 H       0.083838    -2.131167    -1.409407      20.60
 C       2.286698     0.062210    -0.248820      22.39
 C       3.743146     0.435313    -0.663547      97.92
 H       3.829688     0.395970    -1.695250      27.28
 O       3.806908     1.938648    -0.427010     173.37
 H       4.077208     2.285127     0.544760      20.81
 C       4.854672    -0.288045     0.316739      82.10
 H       4.699773    -0.001543     1.357402      26.87
 O       4.560685    -1.767540     0.338614     293.38
 H       4.634694    -2.087440    -0.534352      30.62
 C       6.326660     0.033991    -0.084745     101.54
 O       6.812500     1.477064    -0.020138     209.40
 H       6.763174     1.748035     0.936462      28.43
 H       6.473770    -0.432747    -1.042253      30.37
 H       6.839795    -0.808333     0.443013      30.02
55
name= lig-ACN-Water-frame_581
 C      -3.093492     0.115589    -3.041877      58.84
 H      -2.817594    -0.930475    -3.476138      22.63
 C      -3.798218     1.672997    -1.312494      49.98
 H      -4.297382     1.729276    -0.194395      20.88
 C      -3.692390     2.853443    -2.183265      23.76
 O      -4.136090     4.121528    -1.929022     217.22
 C      -4.544036     4.415773    -0.486030     106.77
 H      -5.429193     3.747155    -0.067859      25.70
 H      -4.973743     5.317157    -0.092206      25.79
 H      -3.648250     4.128724     0.241086      25.89
 C      -3.123295     2.602750    -3.442269       0.93
 O      -2.721515     3.556925    -4.381349     151.57
 H      -3.020621     4.314359    -3.952275      27.58
 C      -2.799251     1.216097    -3.865641      40.31
 H      -2.547363     1.063937    -4.910685      24.12
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 C      -3.514291     0.323090    -1.742575       7.65
 C      -3.747398    -0.932776    -0.683213      72.25
 H      -4.401116    -1.755605    -1.146863      25.34
 O      -4.565289    -0.258582     0.465443     128.86
 H      -3.791677    -0.007987     1.119703      25.03
 C      -2.583288    -1.842903    -0.338781      98.76
 H      -2.199969    -2.225726    -1.308339      25.99
 C      -3.078937    -2.982679     0.485155     119.10
 O      -4.142233    -3.709014    -0.334286     181.76
 H      -3.731849    -3.892528    -1.106766      35.36
 H      -3.723026    -2.845400     1.331611      25.70
 H      -2.324648    -3.659800     0.375411      28.02
 C       1.675079    -1.029444    -1.052645      53.39
 H       2.188278    -1.352900    -1.920826      22.59
 C       1.527161     0.714116     0.797709      48.96
 H       2.021480     1.329076     1.379713      24.65
 C       0.228853     0.386495     1.001616      -5.88
 O      -0.627613     1.148568     1.936710     201.47
 C      -0.832016     2.482482     1.613010     125.49
 H      -0.015266     2.850430     1.189244      27.48
 H      -1.692583     2.658823     0.832872      26.27
 H      -1.340004     2.705266     2.548815      27.09
 C      -0.310417    -0.696552     0.167757      -5.51
 O      -1.635349    -0.971462     0.459959     133.62
 C       0.388064    -1.372871    -0.831558      68.76
 H      -0.252287    -1.999228    -1.278229      24.20
 C       2.298230     0.019993    -0.337642       0.30
 C       3.711478     0.505646    -0.606851      96.78
 H       3.933388     0.312153    -1.614023      29.48
 O       3.859208     1.884138    -0.326310     233.00
 H       3.873786     1.969741     0.646249      26.37
 C       4.884904    -0.220118     0.332261      79.29
 H       4.689370     0.259342     1.333208      28.08
 O       4.555911    -1.581489     0.252639     314.07
 H       4.601477    -1.808884    -0.670513      33.52
 C       6.390208     0.018692    -0.112267     112.02
 O       6.738721     1.325844    -0.054875     255.48
 H       6.931393     1.677055     0.826268      30.41
 H       6.434007    -0.111487    -1.150549      30.75
 H       7.146782    -0.407498     0.555298      29.21
55
name= lig-ACN-Water-frame_582
 C      -3.061627     0.154940    -3.049298      40.28
 H      -2.970894    -0.877859    -3.503695      26.28
 C      -3.771062     1.669197    -1.256636      52.57
 H      -4.297491     2.005718    -0.216467      15.95
 C      -3.598169     2.728200    -2.148476     -43.90
 O      -4.188390     4.167447    -1.943512     126.67
 C      -4.486384     4.398713    -0.497781     114.47
 H      -5.564380     3.931421    -0.299786      24.01
 H      -4.404156     5.399058    -0.758257      24.23
 H      -3.628243     4.121943     0.270885      24.83
 C      -3.060518     2.554202    -3.470726      14.93
 O      -2.732873     3.558007    -4.411080     121.15
 H      -2.924087     4.497208    -4.296713      24.10
 C      -2.844623     1.286741    -3.876109      71.29
 H      -2.599185     1.161684    -4.867196      26.68
 C      -3.528619     0.327968    -1.657952     -36.73
 C      -3.866723    -0.820946    -0.739404      86.32
 H      -4.616918    -1.419768    -1.251343      27.59
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 O      -4.539571    -0.456994     0.483660     170.02
 H      -4.113854     0.041721     1.188203      26.63
 C      -2.605076    -1.651889    -0.245922     116.10
 H      -2.067509    -2.026240    -1.180902      26.45
 C      -3.093913    -3.090450     0.374611     126.60
 O      -4.099084    -3.701072    -0.354535     261.79
 H      -3.796765    -4.216729    -1.141415      28.87
 H      -3.324739    -2.767429     1.414174      26.60
 H      -2.239030    -3.610075     0.736196      28.27
 C       1.781884    -0.967847    -1.156477      52.55
 H       2.437076    -1.602136    -1.765492      17.32
 C       1.616713     0.615681     0.720997      54.28
 H       1.963460     1.468592     1.211091      21.80
 C       0.194844     0.354922     1.029393       7.24
 O      -0.597810     0.976786     2.031259     161.62
 C      -0.916416     2.546744     1.660000      91.81
 H      -0.049810     3.025939     1.354979      27.87
 H      -1.671838     2.535424     0.873701      26.78
 H      -0.988239     3.298789     2.498226      25.62
 C      -0.336389    -0.591659     0.095933       7.30
 O      -1.658828    -0.921537     0.455857     189.35
 C       0.333917    -1.327590    -0.966922      67.39
 H       0.069717    -2.123476    -1.515630      22.38
 C       2.296104     0.038575    -0.269062      33.74
 C       3.784734     0.528775    -0.468985      98.39
 H       4.045255     0.405350    -1.497918      27.11
 O       3.897753     1.951165    -0.273869     246.35
 H       4.059048     2.240044     0.603993      28.32
 C       4.818162    -0.140564     0.260087     112.74
 H       4.837901    -0.046349     1.382330      26.99
 O       4.576020    -1.525142     0.216294     314.52
 H       4.651371    -1.906496    -0.736768      27.56
 C       6.363684    -0.084516    -0.148947      96.83
 O       6.748635     1.417415    -0.091664     232.85
 H       6.795184     1.663275     0.877501      29.09
 H       6.544332    -0.514142    -1.067927      34.31
 H       6.773029    -0.941455     0.413578      32.27
55
name= lig-ACN-Water-frame_583
 C      -3.089377     0.182003    -2.958401      61.48
 H      -2.979444    -0.841546    -3.282245      24.52
 C      -3.770067     1.717315    -1.261943      74.68
 H      -4.171640     1.802087    -0.180575      21.06
 C      -3.605928     2.835816    -2.169985      23.22
 O      -4.123940     3.972146    -1.909372     228.88
 C      -4.426882     4.527700    -0.622219     112.70
 H      -5.517099     4.232055    -0.203984      24.40
 H      -4.417243     5.509212    -0.317578      25.09
 H      -3.744505     3.932675     0.111350      25.39
 C      -3.001538     2.623008    -3.474006      -0.99
 O      -2.777751     3.575304    -4.423805     179.78
 H      -2.928838     4.430399    -3.829973      17.95
 C      -2.878173     1.217665    -3.928714      43.47
 H      -2.443827     1.039738    -4.841432      27.49
 C      -3.508773     0.437143    -1.665819      59.65
 C      -3.892777    -0.735031    -0.722634     105.37
 H      -4.478145    -1.416490    -1.261451      28.53
 O      -4.604416    -0.610853     0.506445     143.25
 H      -4.093480    -0.048189     1.090341      25.51
 C      -2.621261    -1.642138    -0.461807      63.86
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 H      -2.050269    -1.733759    -1.483271      24.67
 C      -2.989014    -3.054024     0.451163      92.54
 O      -4.102355    -3.741473    -0.392985     145.19
 H      -3.486528    -4.096694    -1.265155      25.99
 H      -3.670377    -2.870890     1.295823      23.86
 H      -2.158690    -3.756741     0.339868      24.50
 C       1.763503    -0.907131    -1.122047      35.92
 H       2.274349    -1.474449    -1.970275      23.95
 C       1.539114     0.668027     0.778681      46.64
 H       2.127631     1.437725     1.358858      20.08
 C       0.226712     0.318649     0.922322       8.31
 O      -0.530713     0.913492     2.040856     150.62
 C      -0.857240     2.486358     1.698972      92.92
 H      -0.115131     2.836835     1.059752      27.18
 H      -1.724693     2.498662     1.147593      28.20
 H      -1.278659     2.711591     2.786776      23.88
 C      -0.469213    -0.611866     0.042633      -5.99
 O      -1.755593    -0.844087     0.552824     132.19
 C       0.434712    -1.186248    -0.975813      65.42
 H      -0.078839    -1.882831    -1.565276      24.47
 C       2.427147     0.012704    -0.283079      16.78
 C       3.777764     0.634133    -0.495701      85.23
 H       3.901954     0.547821    -1.585326      24.16
 O       3.940302     2.097106    -0.279512     210.88
 H       3.999033     2.389515     0.692345      25.18
 C       4.907750    -0.241680     0.325826      84.67
 H       4.775679     0.261795     1.361385      26.18
 O       4.563193    -1.685185     0.200971     249.86
 H       4.548586    -1.810483    -0.887096      26.02
 C       6.275196    -0.036269    -0.176407     120.01
 O       6.822823     1.397899    -0.118276     247.17
 H       6.650080     1.789763     0.784285      31.99
 H       6.424676    -0.199374    -1.134016      33.57
 H       6.934789    -0.384022     0.614220      29.47
55
name= lig-ACN-Water-frame_584
 C      -3.118260     0.167935    -2.959210      65.77
 H      -2.885761    -0.800894    -3.250408      26.67
 C      -3.773943     1.834416    -1.240155      72.69
 H      -4.236532     2.158467    -0.337768      21.57
 C      -3.553850     2.743054    -2.214445       5.33
 O      -4.105852     4.093327    -1.943386     167.33
 C      -4.375465     4.553784    -0.576353     118.91
 H      -5.564358     4.394589    -0.484949      24.79
 H      -4.081096     5.498102    -0.840696      25.35
 H      -3.799305     4.101019     0.283622      25.31
 C      -3.029767     2.514045    -3.478325      12.73
 O      -2.848240     3.647408    -4.367965     136.93
 H      -2.919085     4.715706    -4.116810      23.10
 C      -2.840046     1.208174    -3.862885      55.35
 H      -2.582396     0.946056    -4.868774      24.01
 C      -3.536284     0.462190    -1.618621     -44.11
 C      -3.836124    -0.866533    -0.774497      73.55
 H      -4.484125    -1.357112    -1.351294      25.65
 O      -4.623377    -0.635948     0.522399     113.04
 H      -4.049485    -0.355621     1.345920      23.59
 C      -2.657561    -1.702344    -0.442993      99.58
 H      -2.085288    -2.114117    -1.403834      22.41
 C      -3.001304    -2.937459     0.231902     110.29
 O      -4.023492    -3.779522    -0.417022     244.63
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 H      -3.732818    -3.921457    -1.452632      27.38
 H      -3.104521    -2.684088     1.314836      26.11
 H      -2.025949    -3.506995     0.498559      25.34
 C       1.757381    -0.816240    -1.053255      35.92
 H       2.280669    -0.994926    -2.064824      15.08
 C       1.607446     0.663798     0.732725      61.19
 H       1.774833     1.311008     1.695266      23.54
 C       0.211602     0.360726     0.909481       9.94
 O      -0.430061     0.945650     1.928352     260.66
 C      -0.853569     2.189754     1.782319     145.49
 H      -0.088382     2.947566     1.470976      25.73
 H      -1.690034     2.310967     1.264594      28.78
 H      -0.785975     2.802401     2.849089      25.16
 C      -0.445173    -0.573942     0.140162      16.53
 O      -1.831774    -0.840522     0.463871     162.18
 C       0.292772    -1.126545    -0.902165      62.24
 H      -0.052261    -1.759623    -1.754385      23.29
 C       2.376072     0.161773    -0.200662      19.53
 C       3.829202     0.688389    -0.540357      83.25
 H       4.230374     0.512573    -1.585333      25.49
 O       3.994856     2.110720    -0.335063     244.13
 H       3.876644     2.468237     0.660211      23.02
 C       4.809443    -0.309571     0.314380      68.52
 H       4.663810    -0.379341     1.499365      24.23
 O       4.574302    -1.757886     0.219527     245.13
 H       4.698363    -2.219807    -0.784471      25.53
 C       6.414233     0.095209    -0.133911     111.86
 O       6.861123     1.392441    -0.150006     253.48
 H       6.555736     1.922202     0.609900      29.35
 H       6.361702    -0.247684    -1.040970      31.51
 H       7.080979    -0.766664     0.128923      30.46
55
name= lig-ACN-Water-frame_585
 C      -3.115918     0.159182    -2.903001      55.07
 H      -3.047360    -0.832177    -3.223191      25.09
 C      -3.794120     1.749523    -1.185048      69.42
 H      -4.221198     1.947843    -0.295826      22.98
 C      -3.618231     2.875488    -2.156332     -20.82
 O      -4.016520     4.162129    -2.028930     240.51
 C      -4.340824     4.648266    -0.614050     101.48
 H      -5.477115     4.599638    -0.270212      26.02
 H      -4.133402     5.660626    -0.419056      25.68
 H      -3.746673     4.154247     0.145234      27.69
 C      -3.081913     2.602827    -3.543275     -20.56
 O      -2.910241     3.632568    -4.329797     128.30
 H      -3.136497     4.363665    -3.603557      15.25
 C      -2.797236     1.213874    -3.856908      44.10
 H      -2.542514     1.000595    -4.952186      20.77
 C      -3.572683     0.369256    -1.556758      24.06
 C      -3.935146    -0.848308    -0.762994     106.76
 H      -4.523448    -1.483645    -1.228691      27.10
 O      -4.554790    -0.616792     0.453635     221.36
 H      -3.846687    -0.362909     1.145029      24.82
 C      -2.595009    -1.667736    -0.517837      77.87
 H      -1.994834    -1.747780    -1.536628      21.86
 C      -2.955277    -3.020341     0.202103     106.12
 O      -3.945130    -3.776378    -0.427513     288.51
 H      -3.669643    -3.958262    -1.306916      31.93
 H      -3.612815    -2.847568     1.091226      22.65
 H      -1.967668    -3.647698     0.154112      22.43
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 C       1.620402    -0.642244    -1.041734      36.06
 H       2.116840    -1.238515    -1.893177      21.68
 C       1.601615     0.751581     0.869385      38.51
 H       2.232731     1.535583     1.498532      20.09
 C       0.257740     0.354787     0.882209      10.60
 O      -0.371926     0.849917     2.015890     169.31
 C      -0.857818     2.274252     1.885959     107.28
 H      -0.146606     2.690580     1.202078      24.62
 H      -1.728551     2.267173     1.405529      26.54
 H      -1.152130     2.523576     3.099880      22.46
 C      -0.482713    -0.628752     0.142847       9.20
 O      -1.795045    -0.855141     0.324226     204.22
 C       0.329709    -1.115997    -0.883825      68.84
 H      -0.171149    -1.918319    -1.561949      19.46
 C       2.368846     0.284575    -0.317775      12.06
 C       3.861684     0.541408    -0.455501      87.40
 H       3.900719     0.381437    -1.615365      24.44
 O       4.066814     2.029836    -0.369610     157.25
 H       4.332602     2.352313     0.626562      23.30
 C       4.875843    -0.327951     0.332800      78.38
 H       4.671518     0.128496     1.467422      24.17
 O       4.612141    -1.765412     0.207453     279.09
 H       4.788493    -1.976115    -0.839047      24.99
 C       6.366856    -0.067892    -0.174879      94.53
 O       6.909144     1.476945    -0.152374     135.34
 H       6.670242     1.858700     0.729871      29.20
 H       6.419369    -0.135105    -1.103275      32.10
 H       7.085267    -0.586280     0.519676      29.27
55
name= lig-ACN-Water-frame_586
 C      -3.092206     0.193439    -2.916605      57.59
 H      -3.013043    -0.791783    -3.342608      24.70
 C      -3.847399     1.739448    -1.206085      86.57
 H      -4.148073     1.821917    -0.266230      22.15
 C      -3.689601     2.786583    -2.093242     -23.66
 O      -3.957732     4.248066    -1.978276     277.44
 C      -4.284610     4.737731    -0.662410     104.23
 H      -5.305501     4.280144    -0.507149      27.71
 H      -4.080494     5.786769    -0.556227      26.26
 H      -3.678198     4.114668    -0.082310      29.24
 C      -3.173593     2.542618    -3.356499      -9.86
 O      -2.964489     3.653365    -4.315495     272.70
 H      -2.959505     4.640890    -4.081990      17.27
 C      -2.853029     1.241192    -3.790364      47.59
 H      -2.320385     0.974390    -4.808452      25.02
 C      -3.613707     0.425818    -1.688597      31.68
 C      -3.915427    -0.877963    -0.805934      86.43
 H      -4.574723    -1.463546    -1.280120      27.42
 O      -4.525519    -0.548102     0.492781     163.33
 H      -3.938264    -0.005623     0.998437      28.15
 C      -2.602234    -1.641017    -0.654877      72.54
 H      -2.208990    -1.868161    -1.721744      21.93
 C      -2.854468    -3.103604     0.243639      82.53
 O      -3.946717    -3.827005    -0.536405     277.53
 H      -3.544583    -4.230506    -1.258295      32.07
 H      -3.024983    -2.777256     1.327719      23.93
 H      -1.940298    -3.810098     0.532649      22.26
 C       1.616855    -0.604209    -1.191405      39.98
 H       2.327409    -1.131286    -1.878104      20.43
 C       1.658121     0.821304     0.792953      39.08
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 H       1.942848     1.585187     1.625910      19.64
 C       0.253741     0.355246     1.040220      -9.73
 O      -0.430642     0.818393     2.240034     167.67
 C      -0.904071     2.304526     1.953098      94.80
 H      -0.138768     3.100535     1.565500      24.16
 H      -1.749398     2.350982     1.414647      27.19
 H      -0.954059     2.897492     3.071247      23.08
 C      -0.406159    -0.558571     0.116382       4.54
 O      -1.745183    -0.828172     0.312681     146.09
 C       0.383815    -1.175782    -0.929626      55.10
 H       0.131667    -2.133472    -1.543214      19.49
 C       2.301972     0.297104    -0.277381      37.56
 C       3.806179     0.478545    -0.510138      86.40
 H       4.237275     0.130583    -1.569704      23.51
 O       4.147004     1.894056    -0.347236     210.68
 H       4.538020     2.079682     0.536487      23.71
 C       4.946999    -0.281645     0.302676      86.77
 H       5.072218    -0.115016     1.544437      22.83
 O       4.680823    -1.691606     0.226478     313.92
 H       4.548355    -1.998714    -0.730022      26.38
 C       6.354793    -0.029385    -0.188229     111.75
 O       6.874060     1.428730    -0.111809     227.76
 H       7.133128     1.690364     0.822025      28.76
 H       6.542640    -0.565634    -0.951592      35.69
 H       6.998131    -0.614962     0.488967      30.77
55
name= lig-ACN-Water-frame_587
 C      -3.100895     0.170482    -3.037567      66.51
 H      -2.699388    -0.858674    -3.274931      23.45
 C      -3.953859     1.740909    -1.166599      68.67
 H      -4.320969     2.004042    -0.208698      19.81
 C      -3.765666     2.891127    -2.067009     -13.72
 O      -3.889886     4.198284    -1.920637     241.64
 C      -4.240722     4.697886    -0.628123     145.12
 H      -5.285312     4.655051    -0.310222      27.65
 H      -4.224458     5.744757    -0.916264      26.46
 H      -3.669932     4.666407     0.203602      29.50
 C      -3.187215     2.623378    -3.403530      11.34
 O      -2.999405     3.575074    -4.263525     164.47
 H      -2.994884     4.365164    -3.682670      22.55
 C      -2.883770     1.348051    -3.774017      63.09
 H      -2.393451     1.368128    -4.860767      23.21
 C      -3.691916     0.390777    -1.677408      -3.89
 C      -3.862135    -0.808401    -0.824334      67.76
 H      -4.593815    -1.460417    -1.190983      26.73
 O      -4.521747    -0.475842     0.513725     163.73
 H      -3.861542    -0.110679     1.142985      25.77
 C      -2.566352    -1.794460    -0.546059      76.18
 H      -1.941222    -1.964639    -1.443155      22.45
 C      -2.822089    -3.073916     0.126388     104.08
 O      -3.898697    -3.847564    -0.504698     252.74
 H      -3.481379    -4.147775    -1.438968      26.57
 H      -3.385988    -2.821739     1.075317      23.44
 H      -1.763941    -3.577141    -0.028434      21.33
 C       1.795848    -0.669760    -1.256879      39.96
 H       2.232452    -0.880684    -2.194722      23.86
 C       1.481198     0.839140     0.807425      36.59
 H       2.162003     1.465267     1.434460      21.04
 C       0.234622     0.372526     1.215182      17.11
 O      -0.482404     0.936972     2.326907     189.63
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 C      -0.870787     2.311722     2.095204      89.57
 H       0.097205     2.608020     1.512464      24.26
 H      -1.706316     2.361251     1.422914      25.88
 H      -1.252374     2.752714     3.200235      24.11
 C      -0.344841    -0.492834     0.145242     -18.91
 O      -1.704510    -0.808791     0.286388     104.40
 C       0.447785    -1.172428    -0.962044      48.25
 H      -0.124768    -1.933101    -1.573636      19.38
 C       2.332390     0.209755    -0.332014       8.35
 C       3.867789     0.494786    -0.534301      93.28
 H       3.873601     0.303799    -1.724831      23.85
 O       4.183477     1.840841    -0.356422     227.51
 H       4.526052     1.979320     0.502945      29.21
 C       4.887519    -0.282832     0.293211      76.76
 H       4.573519     0.097689     1.484585      24.20
 O       4.747965    -1.680564     0.270117     307.16
 H       4.757546    -1.944196    -0.629913      31.45
 C       6.469465     0.016770    -0.141142     109.88
 O       6.839926     1.314748    -0.098452     210.03
 H       7.248973     1.483267     0.775469      30.78
 H       6.524765    -0.043762    -1.107313      33.16
 H       7.022783    -0.591104     0.557499      31.01
55
name= lig-ACN-Water-frame_588
 C      -3.173359     0.254319    -2.966735      62.83
 H      -2.779824    -0.749665    -3.373554      22.37
 C      -4.047226     1.742838    -1.266659      95.86
 H      -4.478383     1.724860    -0.220551      22.92
 C      -3.758624     2.755042    -2.095143      31.87
 O      -3.851497     4.171388    -1.782782     215.29
 C      -4.273203     4.871296    -0.541221     104.41
 H      -5.039797     4.268976    -0.219426      28.20
 H      -4.442044     5.995821    -0.660426      24.36
 H      -3.501634     4.570927     0.025933      31.43
 C      -3.273881     2.598001    -3.339945       0.51
 O      -2.988765     3.673155    -4.250694     137.11
 H      -3.076535     4.666587    -4.045648      21.92
 C      -2.870409     1.300727    -3.869645      17.92
 H      -2.491969     1.185911    -4.959623      19.21
 C      -3.666655     0.428665    -1.704081     -13.07
 C      -3.866281    -0.843105    -0.684157     100.21
 H      -4.477227    -1.529951    -1.248473      26.15
 O      -4.494320    -0.434905     0.471129     250.04
 H      -3.820683    -0.367263     1.269046      22.65
 C      -2.510635    -1.604279    -0.534410     100.47
 H      -2.158698    -1.815172    -1.524134      24.89
 C      -2.862393    -3.084557     0.114083     106.63
 O      -3.843760    -3.860747    -0.472876     277.72
 H      -3.798983    -3.977989    -1.573663      24.80
 H      -2.932219    -3.030225     1.240214      25.11
 H      -1.878114    -3.750202     0.227022      23.69
 C       1.759787    -0.771951    -1.174161      28.40
 H       2.266530    -1.217934    -1.985238      19.43
 C       1.599416     0.732154     0.778806      37.38
 H       2.009283     1.538856     1.348143      21.83
 C       0.187385     0.353213     1.132499     -17.05
 O      -0.490934     0.928404     2.322967     171.42
 C      -0.808862     2.343163     2.164099      99.36
 H      -0.004079     3.315138     1.986678      23.25
 H      -1.628134     2.508475     1.433324      25.00
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 H      -1.170162     2.722117     3.220827      24.98
 C      -0.326055    -0.593698     0.194596       9.97
 O      -1.672834    -0.828391     0.314582     184.74
 C       0.475138    -1.001164    -0.882208      68.42
 H      -0.092807    -1.480386    -1.646582      24.07
 C       2.349920     0.199355    -0.273833      37.67
 C       3.819788     0.508781    -0.586181      75.34
 H       4.183539     0.275153    -1.719367      22.90
 O       4.183420     1.967123    -0.392724     157.68
 H       4.474452     2.184091     0.600495      24.56
 C       4.898922    -0.299650     0.283875      76.94
 H       4.776074     0.163372     1.465129      24.14
 O       4.786622    -1.753466     0.310983     278.98
 H       4.774102    -1.989961    -0.616819      29.39
 C       6.368287    -0.087120    -0.126797     108.67
 O       6.929212     1.394939    -0.025142     168.21
 H       6.922126     1.703254     0.922071      30.02
 H       6.416274    -0.510083    -1.035801      33.21
 H       7.072063    -0.805008     0.222499      31.47
55
name= lig-ACN-Water-frame_589
 C      -3.150291     0.250901    -2.981541      64.84
 H      -3.161263    -0.847522    -3.272493      23.62
 C      -4.132848     1.623564    -1.248758      69.68
 H      -4.568907     1.941065    -0.183395      22.34
 C      -3.777564     2.864095    -2.040219     -39.13
 O      -3.845015     4.226338    -1.717968     183.05
 C      -4.253004     4.799513    -0.410545     124.95
 H      -5.074587     4.500108     0.085566      28.18
 H      -4.523223     5.840579    -0.876445      23.70
 H      -3.545129     5.082339     0.281321      29.16
 C      -3.221868     2.650860    -3.513982      -7.33
 O      -2.958516     3.763299    -4.256285     107.72
 H      -3.199040     4.509486    -3.588388      19.03
 C      -2.982603     1.309860    -3.878606      76.82
 H      -2.578004     0.980866    -4.842546      23.40
 C      -3.674528     0.375626    -1.636604      32.48
 C      -3.832658    -0.782433    -0.742338     101.28
 H      -4.481065    -1.627165    -1.071343      24.80
 O      -4.538875    -0.426752     0.495390     234.38
 H      -3.951426    -0.073904     1.294622      21.88
 C      -2.553353    -1.514182    -0.551469      78.65
 H      -2.069661    -1.516231    -1.469611      25.11
 C      -2.716030    -3.086700     0.226717      86.27
 O      -3.915531    -3.845509    -0.451548     207.63
 H      -3.352858    -4.090924    -1.362019      25.01
 H      -3.206810    -2.714415     1.129571      23.37
 H      -1.700392    -3.518791    -0.050318      21.48
 C       1.789371    -0.779277    -0.967758      39.55
 H       2.288570    -1.399634    -1.736052      19.42
 C       1.684299     0.677819     0.841872      64.54
 H       2.008511     1.446461     1.463250      23.31
 C       0.348929     0.403644     1.023153       2.99
 O      -0.376645     0.878195     2.164060     143.03
 C      -0.794649     2.445747     2.256408      77.68
 H       0.337757     2.932804     2.110094      21.56
 H      -1.555576     2.697298     1.383118      22.41
 H      -1.312010     2.504866     3.267063      24.17
 C      -0.359646    -0.593179     0.276913       8.16
 O      -1.692171    -0.857268     0.430422     154.38
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 C       0.261126    -1.004016    -0.899375      67.91
 H      -0.107420    -1.714002    -1.574732      21.43
 C       2.451951     0.160603    -0.247691      35.52
 C       3.890562     0.595174    -0.518148      67.20
 H       3.991816     0.347944    -1.695648      21.91
 O       4.115493     2.079590    -0.452968     220.46
 H       4.239654     2.256377     0.549515      25.37
 C       4.937347    -0.306410     0.335978      58.48
 H       4.846972    -0.234462     1.580209      21.76
 O       4.766024    -1.803990     0.331513     252.44
 H       4.581041    -2.170694    -0.623974      25.46
 C       6.374577    -0.056701    -0.175568     106.78
 O       6.973190     1.342762     0.028261     216.25
 H       6.534659     1.646070     0.895408      29.55
 H       6.484766    -0.102898    -1.187446      29.63
 H       6.814112    -0.594792     0.631958      28.86
55
name= lig-ACN-Water-frame_590
 C      -3.207192     0.172061    -2.958948      54.53
 H      -2.851843    -0.729344    -3.475246      21.25
 C      -4.098250     1.842580    -1.261487      63.29
 H      -4.585593     1.808552    -0.161123      18.51
 C      -3.755980     2.844602    -2.101660      26.01
 O      -3.847924     4.203412    -1.658380     225.92
 C      -4.256071     4.804531    -0.346340     101.63
 H      -4.878112     4.165459     0.057154      28.43
 H      -4.777442     5.815702    -0.661028      23.12
 H      -3.367069     4.866341     0.224599      29.03
 C      -3.238624     2.698532    -3.395736       8.27
 O      -2.905685     3.812456    -4.207406     107.61
 H      -3.088737     4.762790    -3.894349      20.81
 C      -3.090870     1.349747    -3.881799      30.25
 H      -2.827801     1.295122    -4.890057      24.20
 C      -3.727498     0.428900    -1.695786     -42.48
 C      -3.915759    -0.795215    -0.685314      76.11
 H      -4.574557    -1.437744    -1.346128      24.58
 O      -4.620708    -0.429572     0.522763     237.50
 H      -3.969371     0.064426     1.038236      27.12
 C      -2.501657    -1.649799    -0.449627      88.51
 H      -1.984522    -1.734998    -1.330954      26.33
 C      -2.771139    -2.922284     0.123130     130.39
 O      -3.829280    -3.756493    -0.400773     305.07
 H      -3.648426    -4.319782    -1.127120      31.14
 H      -2.917209    -2.933173     1.207420      26.11
 H      -1.871208    -3.550499     0.343040      25.05
 C       1.682429    -0.845037    -0.936317      41.47
 H       2.237034    -1.250917    -1.847420      22.64
 C       1.786415     0.781301     0.939393      48.46
 H       2.399518     1.317126     1.621588      21.40
 C       0.395574     0.411685     1.029887      18.99
 O      -0.319580     0.956236     2.042306     220.48
 C      -0.683051     2.323328     2.286088      96.77
 H       0.348741     3.121667     2.540822      22.98
 H      -1.270421     2.871442     1.337156      23.65
 H      -1.231582     2.309969     3.159709      26.85
 C      -0.418588    -0.494392     0.184807     -12.34
 O      -1.739235    -0.819670     0.634389     116.59
 C       0.352675    -1.158433    -0.896602      63.26
 H      -0.108441    -1.957134    -1.432982      21.87
 C       2.500069     0.143566    -0.144186       7.23
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 C       3.945673     0.595297    -0.434722      77.09
 H       4.233315     0.415715    -1.570938      24.41
 O       4.028341     2.097474    -0.433939     250.99
 H       4.121137     2.484210     0.404794      28.12
 C       4.957618    -0.314988     0.329732      87.23
 H       4.840672     0.240097     1.416772      24.02
 O       4.698002    -1.768328     0.308842     233.34
 H       4.747501    -1.970827    -0.777046      25.16
 C       6.483524     0.015782    -0.100280     115.68
 O       6.950267     1.262650     0.081621     258.75
 H       6.801528     1.910361     0.805143      28.12
 H       6.530182    -0.351793    -1.115131      29.71
 H       7.226794    -0.822577     0.077186      29.83
55
name= lig-ACN-Water-frame_591
 C      -3.296936     0.319194    -3.049149      71.32
 H      -2.961082    -0.665445    -3.142924      25.15
 C      -3.993005     1.770971    -1.272322      69.34
 H      -4.399273     2.156007    -0.251724      19.49
 C      -3.759158     2.991109    -2.002863       6.06
 O      -3.849815     4.255957    -1.679400     255.73
 C      -4.227260     4.647732    -0.348232     139.52
 H      -4.864052     4.127854     0.190070      29.61
 H      -4.579240     5.726100    -0.401042      24.44
 H      -3.306906     4.847092     0.253766      27.13
 C      -3.263076     2.747168    -3.335114      -3.98
 O      -2.849855     3.780250    -4.177729     159.94
 H      -3.035680     4.626381    -3.751059      22.90
 C      -3.146279     1.423277    -3.839115      74.42
 H      -2.849720     1.279603    -4.795899      27.97
 C      -3.776556     0.510618    -1.689197      20.64
 C      -3.942662    -0.783950    -0.682625      71.93
 H      -4.631638    -1.689767    -1.058375      24.34
 O      -4.688290    -0.445122     0.498564     212.96
 H      -4.095399    -0.333020     1.244118      27.62
 C      -2.582394    -1.492361    -0.348276      75.18
 H      -2.037203    -1.520614    -1.257804      25.60
 C      -2.766195    -3.002741     0.268646     118.14
 O      -3.823480    -3.684491    -0.374721     299.85
 H      -3.439643    -3.802504    -1.202290      33.27
 H      -3.168092    -2.728876     1.228908      25.80
 H      -1.835255    -3.445541     0.001267      25.93
 C       1.809827    -0.776160    -1.010552      45.77
 H       2.359492    -1.285577    -1.868026      21.18
 C       1.795324     0.727668     0.916604      59.80
 H       2.074244     1.467857     1.696149      20.14
 C       0.395279     0.472841     0.991585       1.62
 O      -0.363593     0.960954     2.086054     205.19
 C      -0.535036     2.338695     2.305967      95.04
 H       0.493261     2.998436     2.728870      21.30
 H      -1.101880     2.841501     1.298988      22.17
 H      -1.313585     2.325136     2.987021      25.01
 C      -0.360085    -0.426706     0.164832      -2.20
 O      -1.658392    -0.814255     0.631845     172.58
 C       0.409285    -1.267416    -0.720918      53.47
 H       0.104661    -1.949471    -1.550651      21.04
 C       2.427604     0.087108    -0.115392      32.14
 C       3.907522     0.530349    -0.476081      68.38
 H       4.067398     0.286957    -1.590460      25.40
 O       3.981278     2.050791    -0.354786     198.63
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 H       4.179657     2.156658     0.607028      27.05
 C       5.084786    -0.233640     0.409220      83.02
 H       4.991574    -0.298870     1.604074      25.42
 O       4.644269    -1.604314     0.267022     250.64
 H       4.625997    -2.049996    -0.745442      24.32
 C       6.484609    -0.156202    -0.099011     103.43
 O       7.018259     1.344591     0.095694     147.74
 H       6.774414     1.351816     1.019826      30.49
 H       6.377266     0.016430    -1.095077      29.65
 H       7.091867    -0.894244     0.542744      29.79
55
name= lig-ACN-Water-frame_592
 C      -3.426421     0.370640    -2.984853      56.21
 H      -3.365280    -0.407567    -3.652916      23.48
 C      -3.965784     1.871448    -1.112179      -0.31
 H      -4.172395     1.746098    -0.059258      16.68
 C      -3.701889     2.939396    -2.027258      -3.40
 O      -3.894244     4.392633    -1.692730     175.98
 C      -4.135408     4.585320    -0.261571     113.50
 H      -4.917696     3.980402    -0.024267      28.79
 H      -4.508250     5.619426    -0.354026      24.29
 H      -3.212566     4.359115     0.413728      27.38
 C      -3.274292     2.784048    -3.366346      22.61
 O      -2.814979     3.773365    -4.145310     165.17
 H      -2.745021     4.662260    -3.720332      22.00
 C      -3.132969     1.522946    -3.858252      47.89
 H      -2.678752     1.414933    -4.795103      21.96
 C      -3.788953     0.426268    -1.643040     -77.43
 C      -3.929613    -0.674686    -0.672278      75.70
 H      -4.296797    -1.561779    -1.412984      21.38
 O      -4.778280    -0.446745     0.513106     193.57
 H      -4.113900    -0.371923     1.289074      23.98
 C      -2.584499    -1.369054    -0.297978      71.47
 H      -2.212445    -1.557653    -1.339609      23.58
 C      -2.742684    -2.887106     0.418538      86.11
 O      -3.859798    -3.659791    -0.417378     208.99
 H      -3.750957    -3.705459    -1.471828      25.89
 H      -2.957794    -3.123812     1.439074      25.01
 H      -1.788546    -3.351232     0.427508      25.93
 C       1.825551    -0.805461    -0.993981      36.84
 H       2.334147    -1.248266    -1.851970      22.25
 C       1.633661     0.670233     0.882602      50.28
 H       2.321693     1.430352     1.401521      19.79
 C       0.290602     0.514988     1.021904      25.98
 O      -0.387442     0.866133     2.157982     181.90
 C      -0.507707     2.489777     2.341194      71.88
 H       0.677867     2.726685     2.738869      20.54
 H      -0.466335     3.040210     1.186962      22.54
 H      -1.212034     2.748320     3.044449      25.28
 C      -0.265624    -0.525134     0.227630      -0.20
 O      -1.551168    -0.774760     0.514085     170.34
 C       0.576910    -1.211157    -0.689593      70.57
 H      -0.105738    -2.010383    -1.146536      21.10
 C       2.528524     0.105131    -0.197091      19.82
 C       3.904666     0.554127    -0.393141      95.52
 H       4.149609     0.307248    -1.462242      25.88
 O       3.973629     1.924841    -0.269842     194.87
 H       4.180600     2.262090     0.722461      23.39
 C       4.986594    -0.229428     0.408158      82.37
 H       5.026980     0.321399     1.454903      25.06
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 O       4.614516    -1.567423     0.258739     256.19
 H       4.539176    -1.636301    -0.781161      26.81
 C       6.495548    -0.066752    -0.133165     103.19
 O       7.059152     1.278386     0.138676     220.46
 H       7.189939     1.737743     1.005512      28.22
 H       6.788287    -0.641107    -1.044462      29.13
 H       7.185705    -0.816235     0.378787      29.26
55
name= lig-ACN-Water-frame_593
 C      -3.531368     0.380291    -3.069813      59.29
 H      -3.588790    -0.648241    -3.267051      24.95
 C      -3.871166     1.887690    -1.057842      78.81
 H      -4.073711     2.208615    -0.150195      19.37
 C      -3.713757     3.017576    -1.945373      -1.68
 O      -3.890254     4.347136    -1.693452     230.61
 C      -4.113934     4.585373    -0.211915     106.12
 H      -4.968528     4.046375     0.093396      29.39
 H      -4.145477     5.501662     0.292004      25.46
 H      -3.205232     4.028170     0.300227      25.43
 C      -3.242955     2.823808    -3.292881     -10.75
 O      -2.769375     3.889946    -4.161615     147.70
 H      -2.811144     4.793192    -3.645959      21.76
 C      -3.122611     1.451917    -3.811309      52.17
 H      -2.863999     1.300730    -4.883819      23.25
 C      -3.796668     0.646615    -1.579587      -9.03
 C      -3.895120    -0.650220    -0.604439      68.82
 H      -4.630825    -1.487832    -1.120720      21.93
 O      -4.842249    -0.444929     0.487283     163.29
 H      -4.363415    -0.085068     1.349414      23.60
 C      -2.510036    -1.509271    -0.282398      82.99
 H      -2.020435    -1.812186    -1.285688      24.19
 C      -2.852175    -2.780839     0.327050     119.59
 O      -3.821606    -3.584396    -0.366378     221.15
 H      -3.254351    -3.838216    -1.283890      25.58
 H      -3.305167    -2.474604     1.253040      25.40
 H      -1.964774    -3.344476     0.265997      26.28
 C       1.916828    -0.901800    -1.022142      33.89
 H       2.376952    -1.334677    -1.855540      17.48
 C       1.721959     0.754413     0.800537      48.92
 H       2.063725     1.399483     1.667957      19.26
 C       0.323274     0.443855     1.111446     -40.97
 O      -0.504417     0.997710     2.265190     125.06
 C      -0.342656     2.463586     2.355691      84.00
 H       0.664175     2.815156     3.022754      21.22
 H      -0.458566     3.034424     1.188670      21.90
 H      -1.243460     2.837620     2.825039      25.12
 C      -0.204369    -0.614200     0.275070       1.39
 O      -1.587082    -0.691275     0.453024     150.17
 C       0.517656    -1.227448    -0.730023      65.84
 H       0.310419    -2.162909    -1.346812      20.54
 C       2.407068     0.143847    -0.178029      34.91
 C       3.932686     0.565653    -0.411475      95.64
 H       4.172341     0.457859    -1.478406      24.23
 O       4.025260     1.997651    -0.189712     280.52
 H       4.050152     2.219320     0.801612      23.92
 C       4.983215    -0.176154     0.324126      72.75
 H       4.810336    -0.089051     1.506101      24.62
 O       4.613641    -1.625244     0.316537     257.61
 H       4.518408    -2.012320    -0.566485      29.59
 C       6.513736    -0.006876     0.003142      96.63
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 O       7.128169     1.240783     0.054595     252.57
 H       7.005731     1.368494     1.034073      29.11
 H       6.495201     0.027199    -1.144647      26.53
 H       6.848240    -0.699575     0.829924      27.80
55
name= lig-ACN-Water-frame_594
 C      -3.609484     0.383845    -2.866434      64.76
 H      -3.378847    -0.580193    -3.342143      22.69
 C      -3.792688     2.053694    -1.061035      52.69
 H      -4.049597     2.042245    -0.094620      20.43
 C      -3.668534     3.091557    -1.997414      10.32
 O      -3.916876     4.389533    -1.552703     211.34
 C      -4.052597     4.516002    -0.161379     114.28
 H      -5.067609     4.456224     0.252432      25.26
 H      -3.832702     5.494828    -0.331848      24.27
 H      -3.275708     3.863057     0.472352      25.31
 C      -3.121242     2.824994    -3.319234      13.32
 O      -2.783356     3.919495    -4.095629     139.41
 H      -3.039869     4.853103    -3.766216      22.05
 C      -3.169715     1.514195    -3.785856      53.82
 H      -2.967271     1.321357    -4.924271      21.82
 C      -3.739526     0.610867    -1.559528      -6.39
 C      -3.904274    -0.622723    -0.649148      65.93
 H      -4.409112    -1.444666    -1.431063      22.64
 O      -4.848452    -0.421627     0.503169     187.02
 H      -4.393163     0.092200     1.218298      24.81
 C      -2.536098    -1.446891    -0.490231      65.58
 H      -2.025597    -1.452242    -1.557938      22.37
 C      -2.906655    -2.764043     0.390694     107.08
 O      -3.810304    -3.540484    -0.374376     288.26
 H      -3.448791    -4.083914    -1.081855      29.15
 H      -3.542782    -2.428545     1.274907      23.23
 H      -2.084989    -3.140664     0.918742      26.47
 C       1.853731    -0.890884    -0.941632      32.43
 H       2.448352    -1.379715    -1.664724      21.19
 C       1.663564     0.868953     0.916998      69.05
 H       2.223281     1.637464     1.329851      18.31
 C       0.417994     0.349705     1.254149      -8.91
 O      -0.483974     1.086899     2.198964     154.44
 C      -0.274561     2.448348     2.367782      91.93
 H       0.730925     2.860195     2.993338      22.08
 H      -0.004611     2.933217     1.171011      21.11
 H      -1.196626     2.883604     2.881093      23.58
 C      -0.273043    -0.636506     0.300747     -24.42
 O      -1.679860    -0.640992     0.464242     101.68
 C       0.518653    -1.333667    -0.793415      49.50
 H      -0.152411    -1.875732    -1.468933      19.53
 C       2.472725     0.150686    -0.235722      28.16
 C       3.840661     0.671590    -0.532556      74.95
 H       4.012608     0.578297    -1.569764      22.93
 O       4.104462     2.130647    -0.123492     278.87
 H       3.993693     2.200703     0.812407      27.32
 C       4.934121    -0.271185     0.429612      79.28
 H       4.767589     0.146253     1.517740      24.64
 O       4.670161    -1.702850     0.362833     285.81
 H       4.733818    -1.869973    -0.539194      29.71
 C       6.403828    -0.063867     0.016379      95.07
 O       7.183470     1.305589     0.082154     198.89
 H       7.124450     1.961767     0.791050      32.58
 H       6.605733    -0.694081    -1.002406      27.80
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 H       7.142200    -0.823762     0.398741      29.53
55
name= lig-ACN-Water-frame_595
 C      -3.453028     0.518045    -2.899381      44.32
 H      -3.622685    -0.533992    -3.306899      25.34
 C      -3.768094     1.962972    -1.099199      74.00
 H      -4.089158     2.376114    -0.165343      17.26
 C      -3.570737     3.065396    -1.970956       9.58
 O      -3.924400     4.367762    -1.535725     241.68
 C      -3.973427     4.698065    -0.049749     108.16
 H      -5.040655     4.427416     0.185599      25.69
 H      -3.657793     5.549419     0.420391      24.38
 H      -3.366246     3.874085     0.583419      22.51
 C      -3.141185     2.903475    -3.263219      24.97
 O      -2.782749     3.911824    -4.105488     187.29
 H      -2.981490     4.781311    -3.708039      22.77
 C      -3.263820     1.529160    -3.717178      61.45
 H      -2.914598     1.241606    -4.823503      18.56
 C      -3.703438     0.680953    -1.441147      45.95
 C      -3.947885    -0.581133    -0.734757      83.28
 H      -4.701330    -1.326647    -1.351949      22.67
 O      -4.771493    -0.418671     0.460955     182.48
 H      -4.250623    -0.019911     1.147661      25.76
 C      -2.625019    -1.301494    -0.439497      82.25
 H      -2.186649    -1.686678    -1.489947      20.56
 C      -2.929397    -2.628037     0.423552      97.09
 O      -3.868820    -3.605616    -0.375610     248.46
 H      -3.357477    -3.814964    -1.113958      31.44
 H      -3.656503    -2.218830     1.233048      22.49
 H      -2.059975    -3.155867     0.696415      25.14
 C       1.774246    -0.865220    -0.859434      70.38
 H       2.274693    -1.283106    -1.763819      17.45
 C       1.698538     0.779153     0.868264      77.31
 H       1.783301     1.697251     1.229489      16.94
 C       0.368839     0.294751     1.240882       4.09
 O      -0.401185     0.994976     2.079513     164.09
 C      -0.177864     2.540697     2.323754      63.36
 H       0.658395     2.508211     3.166005      21.11
 H       0.075122     3.270395     1.254020      19.64
 H      -1.179934     2.982721     2.755458      22.14
 C      -0.298790    -0.580499     0.349375      18.90
 O      -1.701875    -0.608851     0.448503     189.12
 C       0.395583    -1.242547    -0.617677      66.37
 H       0.061773    -1.787245    -1.434722      20.16
 C       2.366550     0.274827    -0.138911      32.88
 C       3.883984     0.759260    -0.456651      81.00
 H       4.209597     0.734370    -1.423952      20.15
 O       4.156234     2.138829    -0.135792     262.80
 H       4.158816     2.234920     0.807643      29.75
 C       4.842880    -0.250435     0.437125      69.00
 H       4.651162     0.030101     1.535239      25.31
 O       4.736417    -1.713852     0.390917     280.69
 H       4.666871    -2.039671    -0.515347      28.51
 C       6.473826    -0.083337     0.013521      83.74
 O       7.129237     1.278289     0.051572     185.24
 H       6.651329     1.501264     0.850387      34.51
 H       6.433218    -0.124525    -1.190684      26.42
 H       6.891842    -0.659564     0.874718      29.60
55
name= lig-ACN-Water-frame_596
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 C      -3.354876     0.496038    -2.871045      60.68
 H      -3.458571    -0.553541    -3.327306      23.79
 C      -3.809016     2.023236    -0.973718      73.63
 H      -4.175445     1.973318     0.136464      18.41
 C      -3.519333     3.120331    -1.770967      -5.87
 O      -3.856618     4.432042    -1.491709     160.48
 C      -3.934377     4.771217     0.028270     103.73
 H      -5.045891     4.802667     0.504075      25.38
 H      -3.617046     5.764114    -0.130081      24.68
 H      -3.253392     3.958236     0.499802      24.95
 C      -3.218091     2.916400    -3.272112      -0.67
 O      -2.777293     3.917394    -4.168748      45.00
 H      -2.738798     4.867742    -3.888721      19.21
 C      -3.206431     1.667279    -3.777558      56.11
 H      -3.142626     1.517101    -4.944070      19.99
 C      -3.671887     0.701442    -1.577411      27.08
 C      -3.978037    -0.534894    -0.700616      90.98
 H      -4.517206    -1.325877    -1.429148      23.43
 O      -4.725424    -0.390402     0.460317     206.41
 H      -4.143560    -0.071930     1.238155      23.11
 C      -2.679946    -1.372099    -0.327500      74.42
 H      -2.019285    -1.549790    -1.314194      19.47
 C      -3.098337    -2.593692     0.343356     115.62
 O      -3.846211    -3.585625    -0.310245     273.61
 H      -3.640418    -3.629384    -1.370719      26.02
 H      -3.339293    -2.534951     1.469535      24.34
 H      -2.068375    -3.022124     0.457787      25.23
 C       1.744356    -0.754900    -0.806039      23.13
 H       2.165128    -1.292468    -1.744503      18.64
 C       1.620837     0.779000     0.934165      58.98
 H       2.055500     1.498541     1.521982      18.15
 C       0.302889     0.378667     1.111703      19.62
 O      -0.419455     1.064988     2.070313     198.99
 C      -0.107876     2.457962     2.296450      81.86
 H       0.652885     2.793146     3.093169      22.87
 H       0.291518     3.060568     1.194697      20.24
 H      -1.262856     2.747114     2.647148      20.18
 C      -0.421486    -0.559003     0.401028      14.13
 O      -1.775736    -0.507882     0.467715     171.78
 C       0.421460    -1.162202    -0.560639      75.68
 H      -0.048519    -1.942628    -0.991951      18.89
 C       2.421427     0.260356    -0.210803      44.25
 C       3.883574     0.669705    -0.343286      95.01
 H       3.999814     0.458991    -1.329184      24.99
 O       4.201298     2.119138    -0.138600     240.92
 H       4.117200     2.343943     0.822227      26.06
 C       4.938754    -0.161302     0.379164      94.74
 H       4.761573    -0.003213     1.454428      25.81
 O       4.733625    -1.667174     0.383161     254.13
 H       4.736444    -1.986773    -0.634056      24.92
 C       6.396494    -0.012217     0.030885     106.01
 O       6.957191     1.213326     0.073473     247.22
 H       7.108588     1.815849     0.848940      30.28
 H       6.648797    -0.711614    -0.996669      28.24
 H       6.992567    -0.851764     0.525648      29.66
55
name= lig-ACN-Water-frame_597
 C      -3.324928     0.549165    -3.034145      43.96
 H      -2.972559    -0.434705    -3.421181      21.26
 C      -3.815235     1.996215    -0.908792      48.29
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 H      -4.198012     2.110856     0.243743      17.76
 C      -3.567320     3.197907    -1.751966       6.89
 O      -3.783102     4.514516    -1.358020     261.00
 C      -3.850871     4.898754    -0.048167     117.35
 H      -4.993657     4.704973     0.410208      25.02
 H      -3.565169     5.968034     0.148367      24.50
 H      -3.125251     4.462327     0.704480      25.93
 C      -3.212720     3.014423    -3.194499     -10.06
 O      -2.806126     3.928774    -4.193826      78.70
 H      -2.968097     4.850478    -3.753814      21.15
 C      -3.140721     1.645543    -3.794746      43.44
 H      -2.936846     1.641757    -4.897806      25.06
 C      -3.674617     0.739953    -1.544186       9.15
 C      -3.886316    -0.525859    -0.735825      73.94
 H      -4.603877    -1.213092    -1.327979      25.42
 O      -4.769603    -0.301984     0.531443     107.00
 H      -4.116168    -0.166766     1.348926      22.52
 C      -2.710770    -1.291971    -0.372720      76.99
 H      -2.208513    -1.660193    -1.395008      22.76
 C      -2.974258    -2.768142     0.441637      96.64
 O      -3.934957    -3.568058    -0.309017     168.75
 H      -3.720074    -3.505066    -1.415867      26.34
 H      -3.675668    -2.502884     1.308683      23.59
 H      -2.015550    -3.317473     0.697191      25.01
 C       1.730035    -0.745376    -0.925920      46.92
 H       2.439051    -1.391494    -1.614983      17.39
 C       1.678997     0.830062     0.934682      50.96
 H       2.199794     1.229927     1.832463      20.19
 C       0.225649     0.561197     1.109587      -5.00
 O      -0.489815     1.137343     2.152205     211.14
 C      -0.143636     2.460999     2.291656      95.64
 H       0.579497     2.572128     3.126837      24.58
 H       0.299860     2.912643     1.141373      20.68
 H      -0.934632     3.291857     2.461981      23.66
 C      -0.460140    -0.478057     0.357817      -5.14
 O      -1.921458    -0.449429     0.551047     164.09
 C       0.384449    -1.223794    -0.582327      59.17
 H       0.141081    -2.024746    -1.180395      22.80
 C       2.420752     0.252839    -0.048978      21.08
 C       3.896110     0.584660    -0.414787      84.47
 H       4.109698     0.533590    -1.407275      27.20
 O       4.182357     2.060183    -0.165887     177.01
 H       4.234245     2.138110     0.881409      24.50
 C       4.957130    -0.229024     0.494399     100.08
 H       5.005616     0.222771     1.448308      27.74
 O       4.678067    -1.580785     0.348696     229.52
 H       4.800992    -1.901421    -0.703771      24.37
 C       6.405743    -0.131404     0.031052      84.46
 O       6.882121     1.294880     0.030505     174.72
 H       6.867002     1.357456     1.017789      30.03
 H       6.437352    -0.237093    -1.208104      27.34
 H       6.912221    -0.669593     0.879801      28.78
55
name= lig-ACN-Water-frame_598
 C      -4.318931     1.382078    -2.556124      31.16
 H      -4.886408     0.401140    -3.032482      19.58
 C      -3.447796     2.384264    -0.505401      56.46
 H      -3.433525     2.392525     0.600955      21.84
 C      -3.090805     3.556219    -1.214646      23.75
 O      -2.779365     4.761812    -0.662618     258.67
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 C      -2.274564     4.913750     0.773504     107.93
 H      -1.282148     4.400008     1.086577      25.10
 H      -2.791217     4.503925     1.530775      27.88
 H      -2.226170     5.997216     0.623870      23.44
 C      -3.271426     3.535014    -2.557793      23.99
 O      -3.208389     4.552625    -3.476414     205.50
 H      -2.671679     5.378724    -3.380268      22.51
 C      -3.850084     2.476459    -3.327756      39.97
 H      -4.144927     2.307754    -4.312652      14.17
 C      -4.095565     1.278153    -1.189619      13.94
 C      -4.459830    -0.027881    -0.392997      77.67
 H      -5.057624    -0.648877    -1.216621      24.15
 O      -5.344498     0.358943     0.653113     171.86
 H      -4.867304     0.636991     1.493213      24.92
 C      -3.300294    -1.033016     0.019840      87.11
 H      -2.876862    -0.897175    -1.043016      25.40
 C      -3.713706    -2.477554     0.316656     113.09
 O      -4.533876    -3.049180    -0.789717     236.81
 H      -3.878100    -3.433944    -1.285098      32.32
 H      -4.403941    -2.282143     1.290646      23.55
 H      -2.703891    -2.889930     0.519896      25.30
 C       1.000493    -1.118943    -0.540098      36.83
 H       1.305817    -1.521904    -1.505277      19.33
 C       1.302556     0.568236     1.253341      54.67
 H       1.744804     1.537816     1.852132      16.61
 C      -0.146738     0.606801     1.538758      -9.27
 O      -0.636401     1.005514     2.785067     201.53
 C      -0.443166     2.303345     3.343258      98.33
 H      -1.070584     2.901320     2.816216      25.90
 H      -0.574781     2.181227     4.665231      22.05
 H       0.668655     2.475658     3.465113      23.80
 C      -1.068186    -0.439074     0.651974      -4.44
 O      -2.419281    -0.402101     0.975545     139.33
 C      -0.450573    -1.111207    -0.345084      76.90
 H      -0.886331    -1.869652    -0.931580      23.36
 C       1.832902    -0.137460     0.191388      25.21
 C       3.277464    -0.098997    -0.286308      87.69
 H       3.163242    -0.645586    -1.196089      24.17
 O       3.594753     1.342157    -0.543719     211.62
 H       3.796344     1.718273     0.375381      25.47
 C       4.332756    -0.756282     0.647235      94.73
 H       4.023349    -0.594306     1.666318      26.32
 O       4.023891    -2.381690     0.667919     210.60
 H       4.401836    -2.618576    -0.219999      27.97
 C       5.832786    -0.851164     0.328772      92.31
 O       6.627054     0.479381     0.262427     221.15
 H       6.821389     0.898220     1.192778      26.63
 H       5.712803    -1.000191    -0.769323      30.10
 H       6.178650    -1.768747     0.846285      30.20
55
name= lig-ACN-Water-frame_599
 C      -4.298521     1.361167    -2.528891      44.85
 H      -4.678725     0.413612    -3.150165      23.87
 C      -3.479185     2.319448    -0.440381      62.16
 H      -3.114376     2.158256     0.672615      17.35
 C      -3.160778     3.520783    -1.097489      11.45
 O      -2.736653     4.774167    -0.590723     297.53
 C      -2.318852     4.920303     0.744981     147.23
 H      -1.310654     4.392959     0.870927      24.41
 H      -3.171382     4.712845     1.209134      29.49
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 H      -2.177271     5.930122     1.115999      23.14
 C      -3.306532     3.504830    -2.630138       5.16
 O      -3.167448     4.628741    -3.438960     258.13
 H      -2.504466     5.186375    -2.972263      25.70
 C      -3.909041     2.464814    -3.243332      50.33
 H      -3.907535     2.734666    -4.204870      19.78
 C      -4.039621     1.279638    -1.140350      48.22
 C      -4.405875     0.014530    -0.509304      79.61
 H      -5.075633    -0.738481    -1.207955      22.78
 O      -5.409059     0.308960     0.647814     137.48
 H      -4.855688     0.486466     1.393714      27.25
 C      -3.281638    -0.895089    -0.092813      95.28
 H      -2.598813    -1.156089    -0.925780      23.26
 C      -3.750398    -2.370717     0.358068     112.42
 O      -4.498085    -3.036111    -0.747974     213.76
 H      -3.898853    -3.285002    -1.434974      31.07
 H      -4.339188    -2.577648     1.365990      25.00
 H      -2.980574    -3.209055     0.469120      24.49
 C       0.970257    -1.081709    -0.465178      44.45
 H       1.356207    -1.571147    -1.326873      17.07
 C       1.121244     0.526147     1.221012      65.08
 H       1.851560     1.152353     1.943372      18.00
 C      -0.223087     0.366791     1.478764      26.93
 O      -0.668630     0.941492     2.755861     205.93
 C      -0.408015     2.300830     3.380651      99.11
 H      -0.774440     3.209201     3.036087      25.30
 H      -1.183391     2.040096     4.390414      20.82
 H       0.650369     2.620767     3.471250      23.89
 C      -1.051388    -0.364864     0.774183      16.97
 O      -2.452421    -0.373852     0.966692     162.52
 C      -0.404017    -1.090662    -0.359957      66.90
 H      -1.015151    -1.333648    -1.204609      20.17
 C       1.810996    -0.149194     0.074215      38.59
 C       3.374891    -0.089037    -0.272291      84.99
 H       3.673309    -0.466565    -1.225355      24.52
 O       3.615586     1.339661    -0.519085     205.45
 H       3.762884     1.796846     0.417526      22.43
 C       4.292047    -0.924063     0.688173      77.54
 H       4.279821    -0.506699     1.733861      23.40
 O       3.957499    -2.296728     0.563036     317.43
 H       3.894710    -2.656065    -0.397037      27.09
 C       5.808789    -0.754540     0.297550     106.91
 O       6.621261     0.429180     0.365677     273.46
 H       6.812316     0.751198     1.308050      27.95
 H       6.070759    -1.251543    -0.683903      29.39
 H       6.406188    -1.384755     1.032082      27.69
55
name= lig-ACN-Water-frame_600
 C      -3.306861     0.575611    -2.841341      62.19
 H      -3.123402    -0.408559    -3.191287      21.94
 C      -3.825394     2.165166    -0.954466      73.96
 H      -4.125687     2.526806     0.024002      20.19
 C      -3.533718     3.242110    -1.753908      -7.78
 O      -3.552243     4.673632    -1.372612     233.38
 C      -3.628472     5.089850    -0.076787     106.03
 H      -4.416852     4.228120     0.420714      23.19
 H      -4.097986     6.189641     0.120476      24.65
 H      -2.755643     4.749798     0.382120      28.43
 C      -3.167839     3.080318    -3.241020     -13.38
 O      -2.987466     4.168116    -4.090606     131.26
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 H      -3.097776     5.191428    -3.856563      19.43
 C      -2.927287     1.719434    -3.618643      71.94
 H      -2.817428     1.504307    -4.617464      27.61
 C      -3.723597     0.792483    -1.515348      26.52
 C      -3.916902    -0.448898    -0.613248     111.21
 H      -4.491210    -1.126089    -1.130908      28.65
 O      -4.721512    -0.012864     0.571318     146.89
 H      -4.187751    -0.002802     1.412161      23.75
 C      -2.775361    -1.315328    -0.344207      85.80
 H      -2.247839    -1.426545    -1.285655      23.38
 C      -2.992671    -2.771547     0.401517     103.89
 O      -4.034276    -3.469602    -0.301145     217.51
 H      -3.750951    -3.464614    -1.300203      27.85
 H      -3.195806    -2.590890     1.469806      25.92
 H      -1.933278    -3.327032     0.469593      24.42
 C       1.657318    -0.809357    -0.814756      39.76
 H       2.230250    -1.470931    -1.401250      21.42
 C       1.577013     0.828184     0.989618      66.01
 H       2.060019     1.531527     1.850725      20.23
 C       0.222344     0.671208     1.239077      16.51
 O      -0.515600     1.468541     2.095454     241.66
 C      -0.416293     2.822624     2.356402     102.92
 H       0.271209     2.870230     3.161263      25.38
 H       0.129786     3.399519     1.529761      24.71
 H      -1.493030     3.265251     2.879645      22.35
 C      -0.452021    -0.268686     0.362831       6.77
 O      -1.831129    -0.683621     0.548064     172.73
 C       0.260988    -0.862404    -0.761634      67.18
 H      -0.356127    -1.525341    -1.502870      17.93
 C       2.259255     0.045201     0.025524      40.14
 C       3.726412     0.479915    -0.302807      82.78
 H       3.845138     0.094853    -1.338040      25.06
 O       3.934952     1.967231    -0.179756     195.29
 H       4.032048     2.135182     0.747573      27.42
 C       4.819081    -0.352714     0.490045      94.90
 H       4.679893    -0.371882     1.469432      28.57
 O       4.508553    -1.794987     0.405179     317.21
 H       4.743753    -2.210308    -0.439614      29.34
 C       6.314001    -0.004023    -0.072781      95.80
 O       6.845470     1.427753    -0.030297     190.05
 H       7.017870     1.905995     0.853228      25.10
 H       6.610369    -0.702921    -1.065202      26.96
 H       6.931383    -0.670665     0.556634      29.96
55
name= lig-ACN-Water-frame_601
 C      -3.252286     0.697541    -2.770749      66.97
 H      -2.984888    -0.316839    -3.071063      24.00
 C      -3.847067     2.166774    -0.870059      70.48
 H      -4.130758     2.012964     0.090766      20.63
 C      -3.429263     3.319981    -1.742459       4.31
 O      -3.524917     4.641686    -1.504681     204.13
 C      -3.571052     4.983107    -0.046221     128.63
 H      -4.403589     4.362725     0.646371      24.16
 H      -3.954766     6.144764    -0.099792      24.30
 H      -2.618047     5.183624     0.408871      27.33
 C      -3.125361     3.067161    -3.167547       4.35
 O      -3.008860     4.106273    -4.151600     215.88
 H      -2.985212     4.843600    -3.570338      26.04
 C      -3.029665     1.776138    -3.706422      48.94
 H      -2.493305     1.667238    -4.649577      22.61
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 C      -3.690139     0.926009    -1.450127      40.66
 C      -4.048602    -0.287713    -0.580872      95.23
 H      -4.749185    -0.782794    -1.103586      28.69
 O      -4.669816     0.035253     0.630575     199.26
 H      -4.043376    -0.178142     1.443138      21.56
 C      -2.679648    -1.332950    -0.349234      89.19
 H      -2.290584    -1.474650    -1.292232      24.67
 C      -2.965423    -2.627385     0.347818     104.55
 O      -4.043764    -3.486292    -0.311911     163.49
 H      -3.969287    -3.281873    -1.402173      26.98
 H      -3.407352    -2.467048     1.289418      26.47
 H      -1.962792    -3.345634     0.357734      23.74
 C       1.600013    -0.789704    -0.857475      36.61
 H       2.081033    -1.364170    -1.569984      21.81
 C       1.611013     0.914883     1.074337      48.41
 H       2.357533     1.614288     1.659710      18.39
 C       0.191978     0.758336     1.121027       7.34
 O      -0.614905     1.419783     2.067263     174.51
 C      -0.434143     2.923551     2.418628      88.71
 H       0.249750     3.265465     3.209354      24.29
 H      -0.425742     3.505909     1.536659      25.18
 H      -1.712792     3.041150     2.607571      19.87
 C      -0.531553    -0.335439     0.363442       7.71
 O      -1.862218    -0.661744     0.703471     169.88
 C       0.192878    -0.842751    -0.732647      73.05
 H      -0.411430    -1.499071    -1.466482      18.80
 C       2.318135     0.090238     0.102833      18.32
 C       3.686740     0.450354    -0.260441      95.80
 H       3.863758     0.439513    -1.389991      25.24
 O       3.823540     1.879676    -0.128980     127.29
 H       4.298335     2.097396     0.773920      25.40
 C       4.728864    -0.345311     0.474815     102.59
 H       4.696052     0.063838     1.385502      28.95
 O       4.599374    -1.795124     0.381665     321.57
 H       4.847373    -2.025931    -0.497855      29.96
 C       6.294963    -0.037749     0.002589      80.68
 O       6.768922     1.363618    -0.078820     249.78
 H       6.686739     1.544126     0.901960      29.24
 H       6.308581    -0.139188    -1.253430      24.45
 H       7.012588    -0.543281     0.622499      29.39
55
name= lig-ACN-Water-frame_602
 C      -3.174840     0.793804    -2.762619      64.50
 H      -3.163493    -0.249084    -3.190438      26.21
 C      -3.766163     2.303355    -0.903795      74.27
 H      -4.068792     2.658296    -0.028684      21.37
 C      -3.412166     3.280566    -1.805153      16.70
 O      -3.501959     4.653016    -1.518806     200.71
 C      -3.525081     5.027211    -0.030713     109.49
 H      -4.168720     4.245875     0.679406      22.46
 H      -4.121253     6.063716    -0.140267      24.21
 H      -2.484170     4.928384     0.288175      24.90
 C      -3.115194     3.075444    -3.166366      31.53
 O      -3.006619     4.038486    -4.085576     193.32
 H      -3.044863     4.972914    -3.976777      23.97
 C      -3.083707     1.787691    -3.653880      56.17
 H      -2.895324     1.571515    -4.808794      22.10
 C      -3.623865     0.962422    -1.386735      23.03
 C      -4.052841    -0.300767    -0.602770      88.57
 H      -4.737422    -0.844338    -1.080059      28.60
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 O      -4.630829     0.081632     0.742093     166.85
 H      -4.009099    -0.014487     1.573178      21.12
 C      -2.730278    -1.196416    -0.320914      66.59
 H      -2.077828    -1.272720    -1.084453      25.29
 C      -3.085897    -2.617926     0.262719     113.76
 O      -3.979452    -3.454524    -0.313849     235.88
 H      -3.881305    -3.466059    -1.336844      28.04
 H      -3.340027    -2.454210     1.279586      26.62
 H      -1.930607    -3.107141     0.383413      23.96
 C       1.503268    -0.658943    -0.780634      33.96
 H       1.958842    -0.828894    -1.697516      23.08
 C       1.555315     0.853315     1.034178      54.33
 H       1.829848     1.819231     1.510188      21.72
 C       0.137198     0.772463     1.088944     -12.20
 O      -0.711400     1.430217     2.084783     171.70
 C      -0.591427     2.891831     2.360925      96.74
 H       0.287165     2.969464     3.075808      23.08
 H      -0.373586     3.403518     1.522687      26.82
 H      -1.605145     3.327995     3.130959      21.87
 C      -0.526750    -0.231479     0.389058      13.09
 O      -1.816875    -0.566829     0.795829     121.48
 C       0.125179    -0.964340    -0.658671      74.79
 H      -0.244071    -1.710778    -1.388362      21.89
 C       2.222318     0.123544     0.059447      32.67
 C       3.702438     0.438943    -0.332731      81.53
 H       3.753258     0.097859    -1.451161      25.01
 O       3.786727     1.888913    -0.035531     122.61
 H       4.381154     2.004678     0.805427      24.39
 C       4.885328    -0.303650     0.511168     113.38
 H       4.744719    -0.235535     1.514893      30.02
 O       4.673303    -1.723162     0.388316     330.71
 H       4.971154    -2.187178    -0.409679      29.69
 C       6.204208    -0.046931    -0.013753     109.93
 O       6.638367     1.302617    -0.054810     234.43
 H       6.989553     1.735885     0.735912      28.46
 H       6.228469    -0.627529    -1.164246      28.44
 H       6.840731    -0.799383     0.438726      32.65
55
name= lig-ACN-Water-frame_603
 C      -3.230752     0.674497    -2.659508      53.67
 H      -3.223795    -0.413981    -3.033015      24.19
 C      -3.656720     2.326188    -0.934854      65.15
 H      -4.080232     2.430637     0.024537      21.45
 C      -3.415073     3.409172    -1.865901      15.07
 O      -3.504336     4.720692    -1.423938     270.13
 C      -3.469937     5.064988    -0.122590     119.46
 H      -4.175438     4.278838     0.498812      22.31
 H      -3.841574     6.095815     0.229232      25.16
 H      -2.457592     5.142496     0.332864      27.05
 C      -3.136272     3.091419    -3.200925       9.11
 O      -2.965632     4.144261    -4.154121      83.26
 H      -3.263035     4.858492    -3.453690      21.31
 C      -3.068172     1.772962    -3.629643      43.64
 H      -3.293863     1.548072    -4.803753      19.82
 C      -3.577729     0.967556    -1.359970      20.77
 C      -3.923402    -0.240551    -0.435341     106.97
 H      -4.485771    -0.862818    -0.983109      28.55
 O      -4.642890     0.115583     0.735986     271.13
 H      -4.059305     0.056882     1.522113      24.41
 C      -2.780019    -1.079230    -0.232679      84.81
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 H      -2.417064    -1.053749    -1.214459      23.84
 C      -3.013816    -2.522461     0.353950      94.93
 O      -3.983129    -3.461266    -0.400421     213.80
 H      -3.534166    -3.578792    -1.174391      32.89
 H      -3.501332    -2.473225     1.307272      25.03
 H      -1.954573    -3.196868     0.331876      22.05
 C       1.428621    -0.615228    -0.871787      48.86
 H       1.890924    -1.176751    -1.698776      22.32
 C       1.386199     0.946468     1.040041      52.68
 H       2.075517     1.529940     1.610551      20.87
 C       0.025450     0.779661     1.205477      33.38
 O      -0.814895     1.430253     2.076107     216.29
 C      -0.619451     2.766843     2.318411     108.07
 H       0.381479     3.058972     2.869352      24.14
 H      -0.687404     3.345211     1.540744      28.11
 H      -1.722162     3.161244     3.005740      22.64
 C      -0.613127    -0.227125     0.382580       8.34
 O      -1.877735    -0.483919     0.778909     153.09
 C       0.138787    -1.042775    -0.526647      64.66
 H      -0.452987    -1.753742    -1.036483      22.36
 C       2.209364     0.196555    -0.000181      15.84
 C       3.690456     0.475963    -0.235074      88.10
 H       4.043931     0.362924    -1.348732      21.97
 O       3.819723     1.944635     0.009289     192.94
 H       4.280653     2.064435     0.816824      26.06
 C       4.781349    -0.331927     0.526943      99.40
 H       4.845091     0.084994     1.510053      26.59
 O       4.698549    -1.738585     0.445563     299.97
 H       4.979994    -1.889262    -0.555045      24.64
 C       6.289523    -0.116870    -0.079893      91.79
 O       6.578769     1.330488    -0.059318     253.16
 H       6.898321     1.402956     0.860523      30.35
 H       6.366606    -0.328417    -1.306328      28.98
 H       7.016106    -0.560435     0.586328      30.35
55
name= lig-ACN-Water-frame_604
 C      -3.305141     0.634469    -2.696249      70.87
 H      -3.228797    -0.444615    -3.054470      23.55
 C      -3.604457     2.299845    -0.930241      64.80
 H      -3.773370     2.504302     0.156455      19.55
 C      -3.405965     3.444163    -1.809915      -1.72
 O      -3.506820     4.817684    -1.522983     187.85
 C      -3.418923     5.131545     0.024189     110.29
 H      -4.137045     4.540423     0.739507      26.22
 H      -3.763207     6.120797    -0.235398      25.38
 H      -2.319686     4.939072     0.315328      25.63
 C      -3.150631     3.142168    -3.230039     -17.16
 O      -2.956481     4.291655    -4.161776     129.59
 H      -3.100277     5.289398    -3.890911      24.53
 C      -3.123333     1.658714    -3.573521      45.49
 H      -2.717615     1.388394    -4.671279      19.46
 C      -3.532637     0.985503    -1.312970      37.64
 C      -3.951078    -0.129199    -0.382640     100.53
 H      -4.655481    -0.611196    -0.910788      26.18
 O      -4.726586     0.193277     0.769323     241.49
 H      -4.214914     0.206219     1.573343      26.97
 C      -2.730899    -1.160287    -0.152380      89.52
 H      -2.105316    -1.379588    -1.020104      23.40
 C      -3.031156    -2.530090     0.412810     100.62
 O      -3.907300    -3.395061    -0.415976     210.97
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 H      -3.662504    -3.379321    -1.366652      29.67
 H      -3.457483    -2.474102     1.432378      25.62
 H      -1.859294    -2.991246     0.641459      23.02
 C       1.449016    -0.705183    -0.914946      46.26
 H       2.052825    -1.390571    -1.620907      20.26
 C       1.408922     1.017670     1.009794      56.17
 H       1.835314     1.553011     1.753932      21.94
 C      -0.007480     0.737220     1.228521       4.65
 O      -0.932685     1.327463     2.083650     166.97
 C      -0.653393     2.809075     2.294817      76.30
 H       0.427780     3.033484     2.788939      22.45
 H      -0.795352     3.238117     1.449676      26.48
 H      -1.596125     3.019955     3.245392      21.16
 C      -0.612754    -0.277395     0.464545      24.59
 O      -1.974215    -0.410629     0.726456     186.14
 C       0.093127    -1.007347    -0.447407      69.31
 H      -0.259634    -1.842354    -0.965429      23.82
 C       2.065503     0.297274    -0.049819      -2.45
 C       3.630055     0.592190    -0.144604      90.30
 H       3.647329     0.429587    -1.310294      23.70
 O       3.876960     2.010785     0.072426     171.39
 H       4.246596     2.215859     0.965591      22.98
 C       4.800379    -0.331429     0.514604      82.91
 H       4.840927    -0.152529     1.630110      25.98
 O       4.631481    -1.803726     0.531138     280.04
 H       4.729992    -2.332321    -0.433297      24.24
 C       6.316363    -0.005222    -0.097509      97.87
 O       6.618118     1.370760    -0.063995     253.41
 H       6.715434     1.827682     0.834905      24.80
 H       6.304684    -0.515783    -1.153227      28.11
 H       6.974192    -0.736183     0.424222      30.20
55
name= lig-ACN-Water-frame_605
 C      -3.335694     0.699179    -2.671264      47.17
 H      -3.281729    -0.350002    -3.042695      24.82
 C      -3.529341     2.418020    -0.886833      47.97
 H      -3.649127     2.777366     0.244860      18.61
 C      -3.406285     3.409160    -1.859217      11.95
 O      -3.505479     4.795510    -1.489779     241.39
 C      -3.385947     5.258213    -0.013176     104.82
 H      -4.162450     4.693831     0.637064      26.23
 H      -3.396379     6.256218     0.266272      26.32
 H      -2.293133     4.978386     0.339060      26.17
 C      -3.177196     3.201724    -3.233612      12.08
 O      -2.954666     4.268133    -4.121573     134.25
 H      -3.196168     4.983177    -3.504092      22.62
 C      -3.103721     1.835584    -3.626189      44.00
 H      -2.657728     1.507182    -4.589917      24.05
 C      -3.525195     0.988969    -1.316152      -6.98
 C      -4.039426    -0.237875    -0.487894      58.39
 H      -4.765914    -0.728087    -1.033108      26.09
 O      -4.802700     0.312608     0.862458      66.60
 H      -4.111123     0.303505     1.576526      23.46
 C      -2.845824    -1.205780    -0.173025      64.44
 H      -2.403450    -1.268885    -1.233205      24.54
 C      -3.081523    -2.594305     0.534123     112.14
 O      -3.841794    -3.316458    -0.355271     176.06
 H      -3.461319    -2.963788    -1.289691      26.91
 H      -3.703836    -2.455686     1.467403      24.37
 H      -2.022085    -3.278747     0.718017      23.29
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 C       1.445569    -0.692829    -0.668699      53.18
 H       2.035861    -1.198861    -1.558473      23.46
 C       1.303607     1.032184     1.014748      67.03
 H       1.818456     1.885410     1.217479      23.09
 C       0.010765     0.703253     1.225794      23.79
 O      -0.922836     1.325055     2.131525     194.72
 C      -0.755655     2.747996     2.317025      93.87
 H       0.432673     2.849067     2.588639      22.46
 H      -0.851122     3.313262     1.509171      28.20
 H      -1.442595     3.441921     3.219967      22.03
 C      -0.591687    -0.336225     0.537099       5.62
 O      -1.935952    -0.353468     0.738187      67.46
 C       0.134430    -1.072389    -0.562341      70.67
 H      -0.413038    -1.876929    -0.995723      22.18
 C       2.080481     0.345516    -0.035875      27.94
 C       3.530545     0.629210    -0.183209      70.35
 H       3.913771     0.458213    -1.249545      25.79
 O       3.896828     2.075976     0.196414      98.64
 H       4.202464     2.000753     1.223500      22.62
 C       4.837662    -0.362407     0.524596      62.80
 H       4.809622    -0.045628     1.657153      26.12
 O       4.511885    -1.823914     0.607255     270.45
 H       4.869062    -2.229333    -0.313327      25.12
 C       6.179521     0.008598    -0.061660      96.77
 O       6.719908     1.457363    -0.116283     203.05
 H       6.989902     1.657994     0.849717      25.67
 H       6.261612    -0.102687    -1.134332      28.16
 H       7.004803    -0.499114     0.500172      29.26
55
name= lig-ACN-Water-frame_606
 C      -3.303244     0.940137    -2.709025      56.80
 H      -3.367481    -0.042462    -3.162407      26.91
 C      -3.473155     2.374471    -0.882788      59.40
 H      -3.771627     2.505494     0.310293      20.35
 C      -3.409311     3.494456    -1.779276      18.26
 O      -3.495290     4.811931    -1.408099     252.23
 C      -3.324694     5.269160    -0.109658     112.08
 H      -4.207492     4.975564     0.512821      26.16
 H      -3.376541     6.249438    -0.391476      26.50
 H      -2.348246     4.760718     0.447192      24.89
 C      -3.186132     3.219932    -3.190057       7.52
 O      -2.984736     4.225193    -4.021453     144.22
 H      -3.094495     5.097384    -3.734296      25.48
 C      -3.054690     1.888415    -3.659275      72.67
 H      -3.106602     1.806173    -4.653539      21.64
 C      -3.619474     1.067122    -1.313045      14.37
 C      -4.155021    -0.216094    -0.360872      92.34
 H      -4.859295    -0.816702    -0.913760      28.66
 O      -4.785553     0.339719     0.768856     183.38
 H      -4.225447     0.187343     1.640553      23.08
 C      -2.900532    -1.142248    -0.060189      92.49
 H      -2.427379    -1.514021    -1.067582      26.23
 C      -3.101013    -2.507915     0.647709      97.11
 O      -3.915581    -3.317084    -0.356695     125.31
 H      -3.385079    -3.584600    -1.292748      25.54
 H      -3.740480    -2.438764     1.616875      25.91
 H      -1.974256    -2.960055     1.037561      24.40
 C       1.507047    -0.756963    -0.602675      41.18
 H       2.170027    -1.299966    -1.427853      22.38
 C       1.331408     1.161496     0.966939      63.97
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 H       1.545400     2.139350     1.372455      23.45
 C      -0.040410     0.704599     1.295074     -17.92
 O      -0.879308     1.332285     2.173758     165.26
 C      -0.718450     2.744255     2.316752      97.17
 H       0.334975     3.204008     2.754272      22.14
 H      -1.098159     3.157521     1.480602      28.21
 H      -1.671809     2.675184     3.223277      21.01
 C      -0.606605    -0.436223     0.444710       7.08
 O      -1.973717    -0.415417     0.669387     175.20
 C       0.082780    -1.092333    -0.464334      73.47
 H      -0.245567    -1.732789    -1.291080      24.44
 C       2.119775     0.365596     0.142719      19.17
 C       3.644584     0.650750    -0.170027      99.80
 H       3.661055     0.625971    -1.295288      26.24
 O       3.833266     2.028806     0.300571     175.96
 H       4.416690     2.158902     1.209479      19.67
 C       4.616459    -0.301540     0.626732      81.43
 H       4.733999     0.101370     1.768305      25.96
 O       4.460634    -1.738273     0.607154     298.93
 H       4.806501    -2.173411    -0.199759      29.36
 C       6.197094     0.056055    -0.123978      90.49
 O       6.760839     1.475896    -0.143249     205.51
 H       7.306773     1.626294     0.666215      26.16
 H       6.086919    -0.420264    -1.011186      33.12
 H       6.891301    -0.662407     0.426982      30.68
55
name= lig-ACN-Water-frame_607
 C      -3.335266     0.871285    -2.752859      42.94
 H      -3.405987    -0.150887    -3.099436      24.62
 C      -3.560694     2.377468    -0.793474      58.21
 H      -3.769272     2.683381     0.379177      18.47
 C      -3.369094     3.433121    -1.645037      11.94
 O      -3.492157     4.809823    -1.464715     222.60
 C      -3.311216     5.338033    -0.105414     118.31
 H      -4.150968     5.284351     0.584766      27.43
 H      -2.943958     6.303492    -0.062613      27.86
 H      -2.243758     4.878696     0.323787      23.79
 C      -3.157148     3.292382    -3.032644      15.10
 O      -3.010268     4.315639    -4.042995     203.58
 H      -3.183578     5.212758    -3.597516      20.92
 C      -3.098337     2.015432    -3.613682      68.02
 H      -2.940605     1.688789    -4.534279      29.78
 C      -3.686271     1.061561    -1.370610      11.00
 C      -4.068743    -0.104437    -0.407219      92.19
 H      -4.824435    -0.696461    -0.980029      27.72
 O      -4.816936     0.345922     0.752144     183.57
 H      -4.253091     0.332947     1.607063      22.74
 C      -2.978132    -1.153412    -0.048003      84.41
 H      -2.573731    -1.345402    -1.166701      24.65
 C      -3.258340    -2.443010     0.636932     105.63
 O      -3.977959    -3.343278    -0.244469     197.39
 H      -3.305291    -3.537263    -0.910201      31.17
 H      -3.920380    -2.416216     1.624400      24.31
 H      -2.139171    -2.986293     0.809887      23.43
 C       1.570849    -0.765014    -0.512748      51.19
 H       2.230806    -1.451327    -1.157592      22.59
 C       1.237228     1.213598     0.969530      39.32
 H       1.756978     1.981215     1.629128      20.32
 C       0.037204     0.647270     1.192799      31.87
 O      -0.790494     1.261215     2.191839     137.34
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 C      -0.825635     2.751731     2.396472     105.89
 H       0.276935     3.124873     2.735806      24.96
 H      -0.978260     3.332848     1.486914      26.31
 H      -1.601863     3.291926     3.292652      23.84
 C      -0.655509    -0.306017     0.510391      19.15
 O      -1.997245    -0.410625     0.699898     150.25
 C       0.231408    -1.105774    -0.452507      57.20
 H      -0.338640    -1.778831    -1.132787      24.26
 C       2.132643     0.267342     0.213196       8.72
 C       3.556426     0.671471    -0.013637     109.24
 H       3.851404     0.481923    -1.070645      26.22
 O       3.779751     2.014876     0.305541     218.49
 H       4.423327     2.078089     1.135372      22.95
 C       4.660514    -0.162457     0.605886      86.15
 H       4.365953    -0.094038     1.786165      24.43
 O       4.425129    -1.596859     0.591978     348.73
 H       4.569793    -1.878963    -0.276398      31.54
 C       6.147674     0.057728    -0.086025      98.95
 O       6.754513     1.362126    -0.214372     237.80
 H       6.959146     1.749103     0.679110      28.47
 H       6.106257    -0.124283    -1.042592      32.13
 H       6.906750    -0.611118     0.449897      29.66
55
name= lig-ACN-Water-frame_608
 C      -3.436403     0.814987    -2.723129      76.86
 H      -3.279386    -0.145010    -3.242420      25.19
 C      -3.694031     2.371040    -0.741909      65.77
 H      -3.921559     2.404841     0.402899      19.91
 C      -3.336373     3.506029    -1.670057      -3.89
 O      -3.499141     4.880314    -1.411453     197.74
 C      -3.207079     5.441359    -0.045529     103.54
 H      -4.108608     5.264299     0.430674      28.22
 H      -3.028345     6.466570    -0.195176      26.26
 H      -2.544296     4.563097     0.507877      24.40
 C      -3.100359     3.342414    -3.089890      -4.20
 O      -3.046206     4.397661    -3.965961     137.46
 H      -3.308840     5.350071    -3.507774      19.07
 C      -3.153885     1.942581    -3.503734      42.45
 H      -2.746029     2.103449    -4.452299      21.21
 C      -3.642483     1.088386    -1.340195      28.62
 C      -4.080299    -0.091794    -0.521923      66.90
 H      -4.846198    -0.686153    -1.131604      24.94
 O      -4.862618     0.368518     0.792556     118.13
 H      -4.190585     0.664241     1.376502      28.21
 C      -2.982035    -1.071219    -0.199236      63.79
 H      -2.365758    -1.505332    -1.157126      25.16
 C      -3.414908    -2.437059     0.645586      96.05
 O      -4.069742    -3.406295    -0.143787     194.94
 H      -3.684645    -3.430485    -0.970751      34.94
 H      -4.044612    -2.090137     1.602955      24.04
 H      -2.346152    -2.891086     1.101965      24.80
 C       1.603296    -0.845077    -0.442446      48.90
 H       2.293748    -1.400288    -1.079020      22.17
 C       1.346147     1.043040     0.988331      70.77
 H       1.827470     1.977344     1.496872      21.23
 C      -0.047899     0.819527     1.232485     -23.79
 O      -0.792864     1.286758     2.292233     184.51
 C      -0.808845     2.726503     2.417262      87.18
 H       0.249715     3.059964     2.893683      20.87
 H      -1.133328     3.222861     1.460830      24.63
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 H      -1.761573     2.729474     3.233025      20.73
 C      -0.603699    -0.326504     0.396720     -21.90
 O      -1.977010    -0.367042     0.810683     106.97
 C       0.187023    -1.065185    -0.379627      74.93
 H      -0.085165    -2.035300    -0.799030      23.54
 C       2.111306     0.315573     0.232090      48.00
 C       3.539858     0.667337    -0.001436      97.78
 H       3.535881     0.642511    -1.096524      24.23
 O       3.740915     2.122837     0.266862     253.82
 H       4.074692     2.187642     1.202283      26.15
 C       4.768406    -0.125011     0.692553      95.85
 H       5.238424     0.283308     1.718573      25.13
 O       4.398630    -1.489027     0.532343     318.75
 H       4.603570    -1.893259    -0.383717      27.38
 C       6.046668     0.007078    -0.037601     113.56
 O       6.741002     1.294357    -0.239774     229.26
 H       6.667075     1.782833     0.642992      31.67
 H       5.892409    -0.406458    -0.870042      34.80
 H       6.745256    -0.730164     0.487410      30.74
55
name= lig-ACN-Water-frame_609
 C      -3.434565     0.924817    -2.694359      27.51
 H      -3.478685    -0.185573    -2.980207      25.56
 C      -3.710628     2.485328    -0.919810      74.06
 H      -4.131155     2.740815     0.046527      23.94
 C      -3.414065     3.597028    -1.634984      23.72
 O      -3.470530     4.964289    -1.301178     265.02
 C      -3.236880     5.421853     0.008362     130.65
 H      -4.004256     5.621028     0.602896      28.59
 H      -2.706033     6.381992    -0.196441      26.19
 H      -2.234590     5.064749     0.603174      24.16
 C      -3.165160     3.312378    -2.999023      13.36
 O      -3.056234     4.386924    -3.883562     145.99
 H      -3.218348     5.395291    -3.503501      19.65
 C      -3.101326     1.981971    -3.580189      66.42
 H      -3.127426     1.418215    -4.527829      22.34
 C      -3.675530     1.103276    -1.293147      27.16
 C      -4.203821    -0.078802    -0.441758      72.82
 H      -5.054792    -0.685328    -1.007052      23.45
 O      -4.832106     0.323169     0.693059     171.11
 H      -4.217739     0.778268     1.333142      25.38
 C      -2.887285    -1.111469    -0.111607      80.55
 H      -2.261774    -1.264869    -1.131682      24.25
 C      -3.447973    -2.258753     0.658980      86.23
 O      -4.224120    -3.484693    -0.108541      34.76
 H      -3.781654    -3.426503    -1.086903      30.57
 H      -4.387519    -1.946870     1.273264      24.11
 H      -2.558374    -2.784642     1.311051      24.03
 C       1.579727    -0.884530    -0.450450      39.19
 H       2.094479    -1.577625    -1.028767      24.07
 C       1.322274     1.053913     1.196964      32.45
 H       1.732203     2.031085     1.649831      19.50
 C      -0.059629     0.818807     1.204312      25.82
 O      -0.784769     1.297134     2.341609     212.53
 C      -0.824235     2.693220     2.508678      89.26
 H       0.063258     3.282559     2.940465      23.07
 H      -1.061044     3.222064     1.465538      23.34
 H      -1.768535     3.052710     3.240697      21.88
 C      -0.680190    -0.141733     0.518220       1.27
 O      -2.005996    -0.436901     0.756397     171.36
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 C       0.184094    -1.168410    -0.333682      41.56
 H      -0.304752    -2.021770    -0.770404      22.37
 C       2.175789     0.227945     0.182010      -8.01
 C       3.691988     0.816858    -0.034975      89.32
 H       4.080691     0.598675    -1.027615      26.47
 O       3.693556     2.242081     0.217353     247.57
 H       4.134522     2.459116     1.058725      27.12
 C       4.734645    -0.066097     0.675999      93.90
 H       4.505049    -0.109746     1.855986      24.43
 O       4.368047    -1.476264     0.554612     276.22
 H       4.967914    -1.890494    -0.233042      27.75
 C       6.130615    -0.101498    -0.131787     106.36
 O       6.673210     1.236504    -0.243675     214.78
 H       6.872290     1.640778     0.646595      28.28
 H       6.043434    -0.404698    -1.018647      34.10
 H       6.842800    -0.730061     0.464974      29.74
55
name= lig-ACN-Water-frame_610
 C      -3.370923     0.966669    -2.615702      56.45
 H      -3.543485    -0.020121    -3.202739      23.41
 C      -3.814695     2.537141    -0.800942      70.23
 H      -4.121207     2.758020     0.140201      23.57
 C      -3.466126     3.641460    -1.714300      -1.36
 O      -3.475993     4.970512    -1.244986     239.50
 C      -3.139029     5.543323     0.125131      86.62
 H      -3.962226     5.444572     0.679035      26.73
 H      -2.856705     6.643378    -0.009769      24.52
 H      -2.544974     4.611472     0.569387      24.04
 C      -3.212220     3.338360    -3.089089       8.83
 O      -3.025919     4.346345    -3.892196      99.66
 H      -3.279696     5.205134    -3.404681      20.28
 C      -3.142961     2.010274    -3.556091      48.39
 H      -3.046051     2.232218    -4.702456      18.33
 C      -3.787292     1.202419    -1.333271      39.57
 C      -4.086598    -0.068998    -0.480247      72.03
 H      -4.778011    -0.796157    -1.151117      25.52
 O      -4.870727     0.294932     0.725714     119.33
 H      -4.258834     0.902669     1.301910      25.14
 C      -2.961846    -1.093949    -0.143772      92.77
 H      -2.597550    -1.534510    -1.160686      27.41
 C      -3.596304    -2.319889     0.665949     108.71
 O      -4.271268    -3.397998    -0.077538      78.23
 H      -3.673979    -3.628975    -0.957034      28.20
 H      -4.322902    -1.714865     1.321833      26.66
 H      -2.890444    -2.857724     1.423455      25.74
 C       1.512129    -0.860600    -0.454720      35.28
 H       2.106839    -1.497738    -0.993065      22.60
 C       1.423455     0.992095     1.136031      60.84
 H       1.915502     1.645265     1.880686      22.50
 C       0.002394     0.781286     1.356081      -7.91
 O      -0.772181     1.287079     2.378221     182.11
 C      -0.871688     2.813958     2.582027      79.03
 H       0.144196     2.986461     2.980824      23.71
 H      -1.045517     3.391616     1.539707      23.97
 H      -1.751784     2.940171     3.330357      24.25
 C      -0.683260    -0.273358     0.454937       6.51
 O      -2.038661    -0.440858     0.768397     170.57
 C       0.103046    -1.086265    -0.188310      71.89
 H      -0.392294    -1.846073    -0.743431      26.48
 C       2.212915     0.341340     0.249712       5.33
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 C       3.682835     0.861145    -0.133121      87.24
 H       3.697036     0.907701    -1.225854      26.14
 O       3.701758     2.304496     0.211349     214.46
 H       4.380317     2.416984     0.954291      24.98
 C       4.726089    -0.165905     0.624692      95.36
 H       4.918988     0.406919     1.646834      26.26
 O       4.310411    -1.533598     0.588332     301.75
 H       4.693106    -2.111009    -0.201244      26.34
 C       6.199145    -0.115446    -0.071026     117.34
 O       6.658733     1.242931    -0.228786     222.60
 H       7.257474     1.404041     0.512114      29.08
 H       5.965349    -0.386679    -0.930383      37.15
 H       6.986295    -0.801132     0.273078      32.50
55
name= lig-ACN-Water-frame_611
 C      -3.379545     0.996568    -2.722785      38.47
 H      -3.152029    -0.124464    -2.955611      22.78
 C      -3.906173     2.569146    -0.722267      73.85
 H      -4.015545     2.674458     0.243350      21.96
 C      -3.541556     3.607797    -1.570373       8.95
 O      -3.485724     5.028906    -1.272235     212.77
 C      -3.142704     5.435220     0.170089     111.98
 H      -3.991100     5.559943     0.656415      29.15
 H      -2.659722     6.519706     0.018753      25.96
 H      -2.223025     5.031429     0.776552      24.34
 C      -3.263320     3.412952    -2.992507      20.42
 O      -2.976493     4.419574    -4.023392     212.67
 H      -3.209460     5.327266    -3.803391      22.57
 C      -3.210199     2.107546    -3.518427      55.52
 H      -2.665089     1.708692    -4.493653      21.85
 C      -3.812745     1.259089    -1.308575      12.38
 C      -4.058211    -0.018880    -0.540037      72.71
 H      -4.945286    -0.552966    -1.179992      23.92
 O      -4.910110     0.258919     0.757277     117.31
 H      -4.448679     0.830281     1.352952      27.11
 C      -3.067160    -1.127334    -0.176019      61.23
 H      -2.377492    -1.447397    -0.974076      23.60
 C      -3.715947    -2.341787     0.747884     110.77
 O      -4.298806    -3.293729    -0.084711     191.95
 H      -3.645555    -3.576507    -0.656268      33.93
 H      -4.545672    -2.119506     1.479047      24.37
 H      -2.750472    -2.645576     1.198252      25.55
 C       1.523270    -0.690278    -0.398592      41.10
 H       1.963509    -1.270320    -1.158284      23.05
 C       1.413518     0.988055     1.194437      45.17
 H       1.912087     1.710892     1.780176      21.59
 C       0.047703     0.652239     1.410785      26.89
 O      -0.782495     1.352987     2.415607     171.67
 C      -0.793078     2.758852     2.640721     108.19
 H      -0.040805     3.332736     3.105281      26.01
 H      -1.192771     3.416669     1.652878      21.74
 H      -1.690214     2.886294     3.340759      24.10
 C      -0.679158    -0.222770     0.671497       3.64
 O      -2.045875    -0.413347     0.796097     103.15
 C       0.173519    -1.099938    -0.262442      64.56
 H      -0.091545    -2.043544    -0.746575      21.02
 C       2.154431     0.302776     0.159872      38.74
 C       3.537259     0.796053    -0.183997      91.12
 H       3.644485     0.740840    -1.274570      24.26
 O       3.806857     2.212965     0.253825     200.96
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 H       4.294702     2.260329     1.172106      22.34
 C       4.819210    -0.194158     0.497471      80.27
 H       4.830276    -0.101018     1.665830      24.63
 O       4.253554    -1.575026     0.665207     350.77
 H       4.407201    -2.023886    -0.175324      29.07
 C       6.148588    -0.123368    -0.115775     122.37
 O       6.731368     1.272320    -0.169205     250.08
 H       7.280156     1.580833     0.600908      28.07
 H       6.231014    -0.486764    -0.977788      35.58
 H       6.755320    -0.712167     0.552901      30.75
55
name= lig-ACN-Water-frame_612
 C      -3.460707     1.075064    -2.602592      65.56
 H      -3.057348     0.104638    -3.017403      22.05
 C      -3.904024     2.526916    -0.755998      67.60
 H      -4.195652     2.690948     0.229234      23.09
 C      -3.605011     3.758819    -1.567896       9.35
 O      -3.463938     5.027444    -1.187575     252.97
 C      -3.158092     5.400544     0.097552      88.54
 H      -3.892700     5.306312     0.873508      26.29
 H      -2.813595     6.525496    -0.059517      23.74
 H      -2.428791     4.570320     0.407038      25.59
 C      -3.303110     3.529264    -3.012555      -1.20
 O      -2.961899     4.451574    -4.028440     156.50
 H      -3.213262     5.301405    -3.699119      22.64
 C      -3.165741     2.165421    -3.497134      43.31
 H      -2.806647     2.116796    -4.621399      21.33
 C      -3.747834     1.222587    -1.300645      41.51
 C      -4.276529     0.018510    -0.436585      79.67
 H      -5.016825    -0.642607    -1.163064      23.34
 O      -4.929858     0.225698     0.709837     203.39
 H      -4.314783     0.616993     1.370960      25.91
 C      -3.041212    -1.081230    -0.024072      97.21
 H      -2.717718    -1.562590    -0.898821      26.99
 C      -3.634449    -2.219145     0.788237     106.23
 O      -4.344289    -3.289161    -0.131866     167.13
 H      -3.672584    -3.534715    -0.794785      31.29
 H      -4.324272    -1.782458     1.509740      25.67
 H      -2.915463    -2.831046     1.291873      27.04
 C       1.491321    -0.733619    -0.579215      30.30
 H       2.123893    -1.177751    -1.365441      17.71
 C       1.370183     1.025859     1.316473      67.03
 H       1.671543     1.980829     1.623450      21.48
 C       0.018559     0.697867     1.538647      -7.12
 O      -0.729921     1.341660     2.446221     217.06
 C      -0.775476     2.757273     2.699233     100.09
 H       0.201835     2.986970     3.010592      23.56
 H      -0.964630     3.258364     1.595409      22.01
 H      -1.560680     2.956430     3.424580      23.60
 C      -0.638782    -0.419541     0.698913       1.63
 O      -2.082553    -0.374572     0.856650     151.54
 C       0.159249    -1.017721    -0.235709      64.37
 H      -0.426325    -1.828740    -0.790056      22.67
 C       2.119609     0.437852     0.220142       3.95
 C       3.591917     0.714861    -0.134370     108.75
 H       3.778965     0.693396    -1.224618      22.95
 O       3.907017     2.035173     0.262016     192.66
 H       4.240989     2.042508     1.214861      25.52
 C       4.570983    -0.222930     0.471043      70.94
 H       4.766215     0.401963     1.428938      23.71
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 O       4.268880    -1.596278     0.677270     323.24
 H       4.415947    -2.103159    -0.102956      29.12
 C       6.249445    -0.094377    -0.173342     101.23
 O       6.790804     1.255607    -0.115642     237.18
 H       6.907328     1.413676     0.872460      29.88
 H       6.386003    -0.471641    -1.026272      32.12
 H       6.776804    -0.652258     0.557461      31.03
55
name= lig-ACN-Water-frame_613
 C      -3.381311     1.116444    -2.646199      30.99
 H      -3.619954     0.174800    -3.127681      24.05
 C      -3.861423     2.646011    -0.823659      50.34
 H      -4.328753     2.847257     0.175642      20.60
 C      -3.624814     3.687425    -1.728449      19.27
 O      -3.547787     5.069234    -1.225774     226.61
 C      -3.111177     5.331053     0.185426      89.33
 H      -4.057161     5.249454     0.644343      24.00
 H      -2.689847     6.413925     0.377929      22.98
 H      -2.236439     4.737031     0.577923      25.51
 C      -3.305743     3.556140    -3.036352      25.58
 O      -2.995785     4.518039    -3.906623     128.52
 H      -3.165758     5.474272    -3.657556      19.99
 C      -3.169046     2.245558    -3.408837      66.28
 H      -3.034434     2.108538    -4.519290      23.25
 C      -3.817162     1.236958    -1.177022     -31.65
 C      -4.217372    -0.104939    -0.426896      71.36
 H      -4.967212    -0.807023    -1.111681      23.22
 O      -5.056366     0.305461     0.796893     129.79
 H      -4.336460     0.527858     1.524429      24.81
 C      -3.027352    -0.996807     0.021650      95.70
 H      -2.472860    -1.170881    -0.810167      28.23
 C      -3.582666    -2.259499     0.789963     112.93
 O      -4.344816    -3.186951    -0.098574      88.51
 H      -3.732616    -3.352629    -1.007241      27.12
 H      -4.396683    -2.029561     1.446397      26.36
 H      -2.813230    -2.673921     1.341712      29.08
 C       1.456688    -0.577343    -0.568831      56.40
 H       1.950692    -1.152714    -1.408543      23.49
 C       1.327763     1.078813     1.273351      57.41
 H       1.803162     1.872437     1.855608      19.60
 C      -0.008906     0.646744     1.532693       8.96
 O      -0.812361     1.251995     2.562510     172.00
 C      -0.637473     2.751870     2.702189      92.03
 H       0.304771     3.075923     3.011252      25.57
 H      -0.945176     3.514649     1.732347      23.59
 H      -1.316949     2.982254     3.416407      24.98
 C      -0.623120    -0.370036     0.819887       3.42
 O      -2.058998    -0.356262     0.907011     157.17
 C       0.080847    -1.049324    -0.294007      45.81
 H      -0.475511    -1.607952    -1.156377      19.22
 C       2.044386     0.339070     0.199631      25.38
 C       3.525769     0.685005    -0.171570      90.71
 H       3.481125     0.677020    -1.289466      23.22
 O       4.012796     1.980419     0.241163     227.09
 H       4.556371     2.034611     1.043263      23.06
 C       4.650992    -0.273691     0.518290      88.86
 H       4.714735    -0.044517     1.624487      24.48
 O       4.295737    -1.623538     0.673093     329.51
 H       4.446804    -2.155703    -0.172477      26.46
 C       6.199462    -0.097294    -0.112144     107.26
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 O       6.805839     1.211561    -0.068507     274.08
 H       6.973802     1.717555     0.769375      28.21
 H       6.149080    -0.269148    -1.033517      33.24
 H       6.786070    -0.852638     0.340590      31.86
55
name= lig-ACN-Water-frame_614
 C      -3.439470     1.090148    -2.544010      65.60
 H      -3.460683     0.163550    -3.014590      25.43
 C      -3.916037     2.618470    -0.789335      52.66
 H      -4.030623     3.030542     0.321133      20.23
 C      -3.600997     3.782177    -1.619470     -26.63
 O      -3.620464     5.101275    -1.298771     145.31
 C      -3.115486     5.257235     0.292569      73.25
 H      -3.888465     5.059844     1.162567      25.19
 H      -2.897482     6.313879     0.049438      24.50
 H      -2.370591     4.526714     0.454017      24.34
 C      -3.254726     3.549275    -3.029697      -7.80
 O      -3.013190     4.667482    -3.859570     123.75
 H      -3.344398     5.576353    -3.437888      18.82
 C      -3.193609     2.169699    -3.517320      53.38
 H      -2.893434     1.839705    -4.474532      23.09
 C      -3.836559     1.285694    -1.288682      50.25
 C      -4.112502     0.028354    -0.316646      48.38
 H      -4.807493    -0.716995    -0.995619      25.53
 O      -5.137972     0.367095     0.843576     118.15
 H      -4.667568     0.617040     1.646229      26.78
 C      -2.948913    -0.983180     0.023162      86.61
 H      -2.556272    -1.339156    -0.834111      29.30
 C      -3.551422    -2.302157     0.787331     118.07
 O      -4.307267    -3.093558    -0.108173     138.33
 H      -3.729887    -3.235303    -0.943509      30.71
 H      -4.136875    -2.009020     1.603449      27.73
 H      -2.692865    -2.890853     1.000579      28.12
 C       1.270483    -0.599741    -0.527745      45.09
 H       1.840899    -0.945803    -1.445172      23.02
 C       1.284490     1.028728     1.201919      44.06
 H       1.941208     1.713377     1.860284      19.14
 C      -0.008605     0.644837     1.585696       6.06
 O      -0.814991     1.251740     2.614520     188.78
 C      -0.540332     2.689189     2.773620      96.51
 H       0.486682     2.904371     2.998846      25.88
 H      -0.845446     2.989948     1.572870      21.90
 H      -1.168039     3.018261     3.447753      28.38
 C      -0.714129    -0.323116     0.714509      13.59
 O      -2.041139    -0.321250     1.023391     154.32
 C      -0.006749    -0.934906    -0.318925      59.84
 H      -0.446722    -1.814703    -0.945268      22.26
 C       2.092378     0.361676     0.246274      19.79
 C       3.510558     0.664929    -0.126659      79.71
 H       3.776157     0.392681    -1.196560      23.08
 O       4.036623     2.040195     0.145766     200.68
 H       4.629196     2.005134     0.925198      22.69
 C       4.792317    -0.325215     0.635826      86.94
 H       4.683979     0.152448     1.572158      26.47
 O       4.339488    -1.721161     0.643020     304.37
 H       4.403126    -2.177822    -0.329405      23.25
 C       6.067646    -0.121384    -0.063745     121.67
 O       6.802217     1.186741    -0.034085     265.19
 H       7.162959     1.335810     0.856353      29.53
 H       5.856955    -0.239133    -0.965724      35.65
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 H       6.725746    -0.893455     0.218345      32.01
55
name= lig-ACN-Water-frame_615
 C      -3.506056     1.058234    -2.662865      48.92
 H      -3.078189     0.154689    -2.765068      26.28
 C      -3.921468     2.698830    -0.730193      60.01
 H      -4.160931     2.480407     0.418155      17.61
 C      -3.578922     3.711183    -1.643764       5.41
 O      -3.647065     5.103444    -1.129332     204.97
 C      -3.167695     5.242304     0.178584     112.17
 H      -4.110030     4.950206     0.912882      24.53
 H      -2.686395     6.155758     0.524720      26.14
 H      -2.320535     4.621009     0.224568      28.57
 C      -3.238489     3.515952    -3.014801       7.77
 O      -3.010371     4.667258    -3.829121     152.81
 H      -3.388753     5.599662    -3.475613      20.46
 C      -3.200901     2.163390    -3.525797      51.27
 H      -2.855211     2.141236    -4.480754      22.41
 C      -3.845384     1.357900    -1.167516     -59.67
 C      -4.155883     0.200063    -0.214594      70.87
 H      -4.817179    -0.492606    -0.948440      20.79
 O      -5.092443     0.396984     0.794640     184.85
 H      -4.707965     0.856692     1.540742      25.91
 C      -2.981731    -0.947343     0.171537     102.14
 H      -2.468419    -1.072254    -0.693998      28.00
 C      -3.371236    -2.251819     0.774049     117.38
 O      -4.340812    -3.049095    -0.205281     169.73
 H      -3.785771    -3.305573    -0.850807      33.62
 H      -3.917205    -2.144179     1.706747      26.36
 H      -2.542277    -2.842042     1.113963      27.15
 C       1.347180    -0.622309    -0.562177      43.99
 H       1.763528    -1.286717    -1.357806      18.33
 C       1.324823     0.979615     1.319085      45.29
 H       1.675568     1.994066     1.830126      21.15
 C      -0.021728     0.653951     1.575400      17.05
 O      -0.698913     1.204128     2.636123     239.54
 C      -0.487040     2.604632     2.782795     118.63
 H       0.576075     2.708240     3.046858      24.46
 H      -0.561142     3.465885     1.825939      23.75
 H      -1.025450     2.972534     3.501178      29.17
 C      -0.790914    -0.147173     0.703499      19.08
 O      -2.106130    -0.369154     1.074341     206.63
 C      -0.153272    -0.850794    -0.307235      76.96
 H      -0.676679    -1.744701    -0.761212      21.61
 C       2.045894     0.357557     0.200967      10.13
 C       3.708723     0.597989     0.000308      87.81
 H       3.734575     0.398422    -1.124485      21.88
 O       3.940730     2.061233     0.013428     228.26
 H       4.461847     2.356135     0.847427      24.09
 C       4.600613    -0.319447     0.755794     103.56
 H       4.883588    -0.260175     1.711295      28.10
 O       4.411545    -1.728180     0.709300     308.52
 H       4.669909    -2.256563    -0.202567      24.23
 C       6.092297    -0.139766    -0.132740     103.53
 O       6.745914     1.087685     0.023482     285.12
 H       7.252919     1.307402     0.838355      29.46
 H       5.944903    -0.280210    -1.048503      36.28
 H       6.697517    -0.950955     0.211192      32.94
55
name= lig-ACN-Water-frame_616
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 C      -3.480030     1.144223    -2.574318      76.07
 H      -3.475566     0.229671    -3.055068      28.09
 C      -3.891214     2.659870    -0.701440      59.14
 H      -4.272116     3.378935     0.104180      13.89
 C      -3.605710     3.754143    -1.565774     -25.55
 O      -3.667520     5.069460    -1.137554     255.67
 C      -3.140415     5.191325     0.222490      98.67
 H      -3.947485     4.885249     1.146148      23.42
 H      -3.083124     6.268741     0.214594      24.93
 H      -2.382857     4.544107     0.494606      26.62
 C      -3.312324     3.571699    -2.941796      12.16
 O      -2.990543     4.528257    -3.818432     147.67
 H      -3.217309     5.425601    -3.504365      18.89
 C      -3.201533     2.231826    -3.445702      61.31
 H      -2.957243     1.939379    -4.413879      24.22
 C      -3.780168     1.352101    -1.234899       8.37
 C      -4.208808     0.097226    -0.289832      57.45
 H      -4.866209    -0.592458    -0.982074      24.23
 O      -5.072907     0.489493     0.838240     149.31
 H      -4.564651     1.122532     1.497715      25.63
 C      -3.083222    -0.778629     0.149603      88.96
 H      -2.612058    -0.970136    -0.770296      30.12
 C      -3.384465    -2.312170     0.711335     109.13
 O      -4.294014    -2.971991    -0.234344     153.44
 H      -3.760502    -3.400102    -0.999252      29.60
 H      -4.059701    -2.249300     1.588550      26.23
 H      -2.365279    -2.734963     0.728216      27.26
 C       1.252266    -0.663241    -0.540871      37.90
 H       1.871098    -1.339792    -1.128120      23.55
 C       1.399052     0.924763     1.317646      48.92
 H       2.059093     1.686781     1.979602      21.81
 C       0.002242     0.713643     1.518445      21.03
 O      -0.645247     1.188348     2.677659     192.32
 C      -0.351517     2.641454     2.903764      97.53
 H       0.651088     2.950054     3.343001      24.51
 H      -0.776518     3.133017     1.806453      23.45
 H      -1.020293     2.830839     3.578552      28.55
 C      -0.807325    -0.062093     0.733338      12.34
 O      -2.114907    -0.333557     1.211713     153.02
 C      -0.053927    -0.795107    -0.335459      72.51
 H      -0.620541    -1.433417    -1.011453      24.59
 C       2.083311     0.323937     0.247375       3.60
 C       3.542681     0.571836    -0.001970      80.74
 H       3.873294     0.209843    -1.039910      24.53
 O       3.839946     2.043648    -0.030427     199.08
 H       4.290954     2.270945     0.856055      23.90
 C       4.753412    -0.322680     0.769846      98.29
 H       4.632792     0.128790     1.641067      28.41
 O       4.407670    -1.745694     0.835103     283.66
 H       4.385765    -2.136331    -0.194668      24.47
 C       6.052621    -0.234126    -0.053101     112.49
 O       6.729099     1.053627     0.041806     268.80
 H       6.997632     1.236818     1.000853      27.89
 H       5.863190    -0.296772    -0.964902      34.41
 H       6.666119    -1.065886     0.273299      31.19
55
name= lig-ACN-Water-frame_617
 C      -3.439987     1.178056    -2.503066      48.99
 H      -3.787067     0.278740    -2.958905      25.29
 C      -3.880003     2.668817    -0.712547      61.49
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 H      -4.238270     2.415343     0.269935      17.55
 C      -3.635042     3.746558    -1.576546      31.32
 O      -3.658416     5.045884    -1.161601     221.12
 C      -3.150967     5.259693     0.368638      78.50
 H      -4.053669     4.910907     1.186535      21.52
 H      -2.857907     6.270558     0.447893      25.18
 H      -2.174268     4.847055     0.312856      28.50
 C      -3.317230     3.538435    -2.909324      18.74
 O      -2.968633     4.497285    -3.860187     169.10
 H      -3.049977     5.368416    -3.510152      22.84
 C      -3.229869     2.253878    -3.347680      61.77
 H      -3.036320     2.262843    -4.445058      21.21
 C      -3.818057     1.295422    -1.134990     -26.41
 C      -4.288049     0.105919    -0.337298      74.12
 H      -4.989700    -0.639009    -0.824557      23.57
 O      -5.076510     0.589016     0.869989     172.76
 H      -4.440094     1.178810     1.303899      29.20
 C      -3.063235    -0.846117     0.125138      67.74
 H      -2.401182    -0.919989    -0.750166      25.73
 C      -3.455490    -2.219419     0.570662     131.70
 O      -4.268048    -2.969042    -0.301265     188.56
 H      -3.590221    -3.160962    -1.170211      24.58
 H      -3.719993    -2.279165     1.679803      25.82
 H      -2.512102    -2.852969     0.756283      25.82
 C       1.332317    -0.654054    -0.477318      41.98
 H       1.683568    -1.107132    -1.394105      21.69
 C       1.446395     0.908724     1.300717      61.99
 H       2.089426     1.292147     2.181305      20.08
 C       0.080663     0.797345     1.584046      -0.76
 O      -0.525483     1.256218     2.745215     220.46
 C      -0.365229     2.649103     3.059132     101.82
 H       0.785351     2.856313     3.244906      23.59
 H      -0.467580     3.395197     2.021408      24.15
 H      -0.953260     2.985185     3.791080      26.62
 C      -0.772245    -0.119986     0.707428       2.47
 O      -2.099530    -0.221394     1.225198     111.81
 C      -0.139171    -0.782362    -0.317761      72.98
 H      -0.570227    -1.446506    -1.018382      25.17
 C       2.082629     0.190209     0.335067      37.92
 C       3.479781     0.521468    -0.152241      84.02
 H       3.397968     0.340290    -1.278287      24.67
 O       3.745351     1.962780    -0.000905     194.99
 H       4.239774     2.166441     0.810847      24.79
 C       4.722602    -0.306844     0.776701      94.51
 H       5.020627    -0.027885     1.690337      28.44
 O       4.371614    -1.710331     0.973567     248.76
 H       4.362533    -2.218292     0.042846      26.59
 C       6.077192    -0.274494     0.039436     111.65
 O       6.726771     0.999245     0.052479     278.37
 H       6.950354     1.430435     0.924498      28.18
 H       5.864345    -0.534521    -0.843312      33.35
 H       6.766942    -1.085799     0.367107      30.61
55
name= lig-ACN-Water-frame_618
 C      -3.522833     1.034772    -2.522169      63.33
 H      -3.197522     0.007402    -2.857527      22.88
 C      -3.916179     2.591887    -0.600340      64.57
 H      -4.023826     3.097634     0.266415      16.75
 C      -3.634423     3.720878    -1.481104     -42.86
 O      -3.604724     5.145313    -0.995958     301.52
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 C      -3.137764     5.359231     0.298757     100.93
 H      -3.941269     4.731915     1.111996      22.34
 H      -3.184033     6.381918     0.569586      25.04
 H      -2.311620     4.675531     0.587148      24.70
 C      -3.241659     3.565724    -2.910117      -3.05
 O      -2.964517     4.537301    -3.868510     158.67
 H      -3.124742     5.496450    -3.518860      21.49
 C      -3.248495     2.175783    -3.363670      51.58
 H      -3.011619     1.833833    -4.462758      21.71
 C      -3.863632     1.279507    -1.170374      21.98
 C      -4.298219     0.165189    -0.204442      86.20
 H      -5.006722    -0.322697    -0.859237      24.17
 O      -5.052626     0.630607     0.851312     227.12
 H      -4.574669     1.058782     1.548528      26.45
 C      -2.990434    -0.796696     0.094688      75.55
 H      -2.482597    -0.897377    -0.962998      24.06
 C      -3.367753    -2.229567     0.616039      92.77
 O      -4.304143    -2.991699    -0.436504     121.46
 H      -3.820200    -3.143436    -1.308698      28.61
 H      -4.243108    -2.050903     1.396428      23.52
 H      -2.349270    -2.747604     0.785149      25.04
 C       1.243395    -0.695814    -0.507277      29.04
 H       1.740463    -1.026938    -1.426050      22.30
 C       1.492965     0.882269     1.466218      53.96
 H       2.030692     1.675003     2.026585      20.69
 C       0.072613     0.754316     1.632894      16.77
 O      -0.462739     1.322262     2.808267     215.85
 C      -0.264872     2.724113     3.150968     104.18
 H       0.809398     2.944202     3.571157      23.08
 H      -0.721217     3.518493     2.318502      22.36
 H      -0.850253     2.703911     3.998546      23.77
 C      -0.726003    -0.065954     0.867354       6.78
 O      -2.135397    -0.143063     1.056607     155.66
 C      -0.113207    -0.830162    -0.290667      60.83
 H      -0.755506    -1.510755    -0.787521      22.50
 C       2.096764     0.085151     0.319114      16.26
 C       3.587166     0.447855    -0.096059      91.92
 H       3.899602     0.125724    -1.141452      24.57
 O       3.678778     1.880232     0.011552     197.06
 H       4.179350     2.097561     0.820514      26.19
 C       4.592867    -0.323982     0.710795     105.62
 H       4.400302     0.263377     1.539153      29.16
 O       4.312062    -1.679537     1.087153     289.73
 H       4.502430    -2.207128     0.338993      31.65
 C       6.132878    -0.330353     0.051741     104.37
 O       6.745467     0.979541     0.003693     266.60
 H       7.049503     1.278961     0.873569      29.54
 H       6.259676    -0.575702    -0.840532      32.68
 H       6.638370    -0.976475     0.825329      28.94
55
name= lig-ACN-Water-frame_619
 C      -3.558810     1.029585    -2.506346      53.58
 H      -3.226723    -0.036365    -2.902477      21.48
 C      -3.900380     2.735535    -0.628112      56.73
 H      -4.167209     2.625394     0.300539      16.67
 C      -3.521532     3.813958    -1.459500      17.89
 O      -3.555794     5.113214    -0.997427     228.18
 C      -3.159705     5.350463     0.410534     127.31
 H      -4.076053     5.062201     1.206872      23.56
 H      -3.085406     6.449815     0.356534      24.44
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 H      -2.025491     5.239354     0.559716      24.12
 C      -3.245727     3.453599    -2.859459      -5.54
 O      -2.975444     4.576172    -3.806262     128.40
 H      -3.271235     5.501155    -3.370931      21.37
 C      -3.255571     2.111218    -3.360655      52.02
 H      -2.797993     2.017634    -4.458497      20.07
 C      -3.913532     1.308952    -1.151448     -45.74
 C      -4.205185     0.143792    -0.188815      79.39
 H      -4.778170    -0.655965    -0.568444      25.08
 O      -5.079072     0.643680     0.943952     154.61
 H      -4.481873     0.990198     1.724708      23.63
 C      -3.032491    -0.720466     0.026227      79.51
 H      -2.576881    -0.905477    -1.085522      23.47
 C      -3.430677    -2.263013     0.525631     107.66
 O      -4.257878    -2.961429    -0.488431     215.85
 H      -3.682538    -3.262874    -1.108453      31.22
 H      -4.071593    -2.177578     1.545719      24.74
 H      -2.700751    -3.082530     1.007455      24.51
 C       1.239252    -0.699548    -0.521563      52.74
 H       1.574605    -1.471291    -1.269802      23.16
 C       1.553932     0.730690     1.434841      56.39
 H       2.076674     1.570844     1.736982      19.94
 C       0.151219     0.732729     1.797352      -0.58
 O      -0.459472     1.370345     2.843097     211.44
 C      -0.205843     2.767094     3.300169     100.54
 H       0.848785     3.288742     3.278581      22.70
 H      -0.780377     3.369947     2.456044      23.16
 H      -0.728895     3.010900     4.207200      23.93
 C      -0.740403    -0.138399     0.832621      12.22
 O      -2.127871    -0.038485     0.925971     184.81
 C      -0.135328    -0.831929    -0.110390      57.85
 H      -0.681135    -1.475605    -0.803113      20.94
 C       2.097591     0.125098     0.330379      30.83
 C       3.499366     0.319674    -0.121089      87.36
 H       3.472218     0.155957    -1.226309      23.71
 O       3.709222     1.824535     0.021674     203.48
 H       4.219398     2.091188     0.864778      24.44
 C       4.663924    -0.296669     0.749934     108.16
 H       4.911618     0.088366     1.692438      27.19
 O       4.238544    -1.681436     1.152605     281.07
 H       4.332207    -2.255975     0.405666      29.94
 C       6.090818    -0.345136     0.189360     106.37
 O       6.789020     0.978697    -0.054515     248.31
 H       7.214482     1.334952     0.789365      27.70
 H       6.023156    -0.944778    -0.550825      33.72
 H       6.788955    -0.934956     0.880745      29.13
55
name= lig-ACN-Water-frame_620
 C      -3.532727     1.116131    -2.464041      39.27
 H      -3.975721     0.053496    -2.827278      22.93
 C      -3.893789     2.665455    -0.686796      89.03
 H      -4.206200     3.005850     0.192170      22.60
 C      -3.444654     3.726049    -1.478781      -4.62
 O      -3.484249     5.076643    -1.057413     208.07
 C      -3.148027     5.502039     0.478010      75.59
 H      -3.805721     4.832980     1.291488      24.66
 H      -3.331735     6.632147     0.537719      24.58
 H      -2.178332     4.844206     0.679769      20.72
 C      -3.257193     3.532594    -2.850001      13.67
 O      -3.008343     4.505199    -3.670223      80.76
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 H      -3.223106     5.388068    -3.279487      18.08
 C      -3.216634     2.189069    -3.311296      53.07
 H      -2.975035     2.045273    -4.438628      21.69
 C      -3.935982     1.407993    -1.158477      24.22
 C      -4.318663     0.161137    -0.201978      62.84
 H      -5.038473    -0.282920    -0.798360      26.55
 O      -5.035069     0.591563     1.037555     179.19
 H      -4.369939     0.839621     1.757316      25.88
 C      -3.000258    -0.825596     0.058803      59.57
 H      -2.412665    -0.836182    -1.014538      22.42
 C      -3.517241    -2.221330     0.500393     113.25
 O      -4.205113    -2.919843    -0.520340     216.51
 H      -3.566579    -3.484232    -1.056497      27.51
 H      -4.245135    -2.093221     1.423773      24.35
 H      -2.396276    -2.644560     0.523793      22.67
 C       1.251870    -0.770352    -0.403013      39.24
 H       1.730146    -1.342049    -1.285819      23.45
 C       1.525482     0.727909     1.452833      55.43
 H       2.176036     1.071962     2.142730      20.42
 C       0.160596     0.637122     1.821585       5.25
 O      -0.455476     1.392379     2.945251     208.59
 C      -0.209660     2.817585     3.271037      99.00
 H       0.888328     2.845839     3.100546      25.08
 H      -0.836240     3.519651     2.675804      25.00
 H      -0.268899     2.817110     4.387806      24.77
 C      -0.729641    -0.062276     0.956506      -0.61
 O      -2.106705     0.073622     0.900530     140.13
 C      -0.080167    -0.920289    -0.120888      63.96
 H      -0.758175    -1.582675    -0.710533      19.96
 C       2.034715     0.024229     0.252519      31.49
 C       3.484794     0.411101    -0.100957      81.50
 H       3.709517     0.022352    -1.116607      25.03
 O       3.762480     1.777840    -0.031895     214.93
 H       4.307089     1.937863     0.840098      22.22
 C       4.696307    -0.359157     0.921153      82.99
 H       4.522780     0.222837     1.819526      27.34
 O       4.226558    -1.680080     1.179184     248.84
 H       4.113275    -2.175498     0.242824      26.71
 C       6.140402    -0.349011     0.255532     103.37
 O       6.782074     0.902854    -0.124415     252.85
 H       7.238391     1.316642     0.701357      26.78
 H       6.183614    -0.749561    -0.615190      32.26
 H       6.757029    -0.899129     1.071965      27.97
55
name= lig-ACN-Water-frame_621
 C      -3.612845     1.190575    -2.456398      44.87
 H      -3.648418     0.158214    -3.140407      23.21
 C      -3.903482     2.706825    -0.557182      62.06
 H      -4.177806     2.915398     0.457166      19.44
 C      -3.430584     3.731926    -1.417206      11.18
 O      -3.389747     5.122636    -1.000103     239.40
 C      -3.158403     5.426238     0.361029     122.82
 H      -4.136065     5.041686     0.985676      24.33
 H      -3.209279     6.634751     0.455529      24.75
 H      -2.018733     5.416201     0.792829      23.39
 C      -3.189076     3.503386    -2.786754       9.16
 O      -3.007297     4.584712    -3.677176     156.53
 H      -3.133188     5.422818    -3.261765      22.39
 C      -3.204231     2.231992    -3.318631      57.19
 H      -3.213705     2.022077    -4.373202      21.83
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 C      -3.931164     1.320754    -1.074265       3.84
 C      -4.413582     0.232883    -0.231097      80.75
 H      -5.104959    -0.384380    -0.645056      24.45
 O      -4.934302     0.488818     1.072493     207.53
 H      -4.226433     0.685356     1.641157      28.83
 C      -3.122228    -0.691198     0.016317      62.74
 H      -2.580178    -1.011877    -1.032642      22.89
 C      -3.384595    -2.136994     0.542994     103.52
 O      -4.217182    -2.892446    -0.574146     144.23
 H      -3.478791    -3.354324    -1.296628      22.67
 H      -4.121616    -2.174560     1.419631      25.33
 H      -2.650629    -2.921509     1.123584      23.69
 C       1.241471    -0.955538    -0.415124      33.37
 H       1.583656    -1.375991    -1.449847      20.11
 C       1.514270     0.694869     1.534362      50.93
 H       2.142576     1.075594     2.249656      23.28
 C       0.066385     0.702587     1.870097       4.12
 O      -0.460453     1.298759     2.987217     213.85
 C      -0.098974     2.725576     3.180366     106.85
 H       0.744766     3.253799     2.774285      25.67
 H      -0.954070     3.245363     2.818513      25.09
 H      -0.282165     2.966985     4.298073      23.71
 C      -0.713258    -0.133275     0.882336       6.63
 O      -2.144279     0.114770     0.965553     112.20
 C      -0.149968    -0.955667    -0.050539      60.90
 H      -0.786878    -1.682093    -0.593938      22.59
 C       2.127569     0.131544     0.404124      -7.03
 C       3.652250     0.331936     0.004016      95.39
 H       3.860978    -0.022852    -1.012032      27.33
 O       3.800123     1.811612    -0.140423     208.01
 H       4.227375     2.302340     0.657423      23.18
 C       4.535766    -0.314242     0.946272      95.87
 H       4.556574     0.133175     1.978797      26.45
 O       4.261429    -1.723936     1.195196     223.91
 H       4.178900    -2.203648     0.253000      27.56
 C       6.180736    -0.382140     0.307683      89.83
 O       6.778410     0.862913    -0.134093     228.04
 H       7.092075     1.435277     0.630461      25.90
 H       6.004646    -1.065633    -0.403124      32.10
 H       6.936767    -0.962403     0.962610      28.59
55
name= lig-ACN-Water-frame_622
 C      -3.685651     1.173467    -2.460110      58.54
 H      -3.445083    -0.012354    -2.657905      21.67
 C      -3.861193     2.688209    -0.459101      66.79
 H      -4.155461     2.609486     0.683612      16.49
 C      -3.435560     3.820680    -1.299619      -0.35
 O      -3.271477     5.096223    -1.038092     258.98
 C      -3.203853     5.486271     0.329290      97.55
 H      -3.906273     4.966996     1.128394      24.37
 H      -3.403404     6.674764     0.207671      23.42
 H      -2.110535     4.992887     0.697903      23.30
 C      -3.113348     3.606979    -2.761764      -2.40
 O      -2.974711     4.655501    -3.690122     185.63
 H      -3.249045     5.560992    -3.317371      26.36
 C      -3.281280     2.248755    -3.306691      62.31
 H      -2.996905     2.182701    -4.283198      21.76
 C      -3.966300     1.467997    -1.090859      15.47
 C      -4.348317     0.096641    -0.179521      92.77
 H      -4.971401    -0.462789    -0.733559      26.21
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 O      -4.892840     0.433654     1.122627     197.23
 H      -4.123555     0.519775     1.781790      22.70
 C      -3.099417    -0.652244    -0.000464      67.61
 H      -2.566233    -0.429649    -1.044389      22.76
 C      -3.449797    -2.131326     0.570011     110.68
 O      -4.181653    -2.803906    -0.515084     150.21
 H      -3.443061    -3.180770    -1.267187      23.24
 H      -4.185639    -1.895910     1.348534      25.22
 H      -2.351521    -2.596663     0.770525      23.93
 C       1.285762    -0.818870    -0.272179      43.84
 H       1.656998    -1.606444    -1.018771      22.65
 C       1.492445     0.653413     1.634377      47.35
 H       1.948134     1.476496     2.118192      22.01
 C       0.091572     0.641631     1.742482       1.39
 O      -0.407745     1.189468     2.984144     216.46
 C      -0.170716     2.674043     3.095514      99.59
 H       0.644318     2.784416     2.514483      27.34
 H      -0.963877     3.162495     2.685783      25.28
 H       0.246228     2.977079     4.190527      22.61
 C      -0.833593    -0.088048     0.911332       0.28
 O      -2.208777     0.054305     0.982780     133.80
 C      -0.120484    -1.007697    -0.031121      56.74
 H      -0.702223    -1.662132    -0.669668      20.76
 C       2.085129    -0.004158     0.428389      28.40
 C       3.557093     0.337711     0.032649      71.93
 H       3.676153    -0.198724    -0.910624      26.62
 O       3.848144     1.852077    -0.282691     170.67
 H       4.250816     2.197411     0.557271      25.48
 C       4.731694    -0.367261     1.023047      82.04
 H       4.700053     0.160163     2.078734      25.57
 O       4.283499    -1.772501     1.196036     277.20
 H       4.400909    -2.245705     0.395716      30.67
 C       6.081479    -0.407892     0.396014     110.36
 O       6.772995     0.828803    -0.135148     236.01
 H       6.943651     1.315477     0.679678      29.72
 H       6.129249    -0.956418    -0.502941      30.60
 H       6.690248    -0.807026     1.260873      28.47
55
name= lig-ACN-Water-frame_623
 C      -3.663583     1.246875    -2.400687      30.21
 H      -3.823392     0.179156    -2.947652      23.01
 C      -3.787617     2.747103    -0.509582      68.22
 H      -4.029040     3.240398     0.595220      15.70
 C      -3.410298     3.740370    -1.376985       8.29
 O      -3.205396     5.143656    -1.055286     269.81
 C      -3.197390     5.554583     0.394645     108.89
 H      -4.141006     5.092538     0.830429      26.23
 H      -3.189732     6.765713     0.680533      23.66
 H      -2.094951     5.322665     0.944798      20.87
 C      -3.221888     3.607597    -2.735845      14.57
 O      -2.914875     4.646917    -3.633767     203.28
 H      -3.264759     5.589745    -3.312350      20.52
 C      -3.311043     2.343551    -3.244218      56.99
 H      -3.006843     2.092050    -4.177395      19.99
 C      -4.058008     1.398627    -1.055070      21.13
 C      -4.255474     0.225334    -0.181874      87.12
 H      -4.959494    -0.389783    -0.592614      23.32
 O      -4.916290     0.380755     1.160982     176.30
 H      -4.293407     0.352989     2.003533      21.81
 C      -2.947692    -0.717025     0.017009      87.11
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 H      -2.312442    -1.072339    -0.896777      21.81
 C      -3.431882    -2.002706     0.473538     125.64
 O      -4.178384    -2.749097    -0.430735     235.18
 H      -3.574087    -3.322146    -1.000034      24.33
 H      -3.894421    -2.066804     1.439304      25.91
 H      -2.506107    -2.726482     0.826151      23.73
 C       1.214122    -0.848522    -0.195597      53.55
 H       1.826626    -1.443031    -0.885324      21.26
 C       1.464007     0.662987     1.545707      58.68
 H       2.119516     1.278676     2.249577      20.74
 C       0.054774     0.540922     1.784349      13.94
 O      -0.404559     1.131247     2.954823     251.74
 C      -0.212135     2.581213     2.929832     108.18
 H       0.513447     2.926582     2.330238      26.52
 H      -1.014118     3.167504     2.767952      26.96
 H       0.030728     2.875768     4.147950      22.06
 C      -0.832417    -0.132631     0.863233      14.48
 O      -2.230916    -0.016328     1.030546     206.00
 C      -0.133749    -0.924360    -0.012544      62.69
 H      -0.558237    -1.663145    -0.629738      21.28
 C       2.145037     0.059763     0.605694      35.04
 C       3.488587     0.366835     0.030627      81.56
 H       3.663358    -0.129782    -0.924095      24.05
 O       3.843465     1.746920    -0.378089     231.56
 H       4.143688     2.227868     0.412199      27.27
 C       4.684905    -0.413090     1.024448      91.25
 H       4.674912     0.170780     2.079267      24.15
 O       4.342680    -1.781303     1.214557     286.97
 H       4.531863    -2.217958     0.389201      30.25
 C       6.188417    -0.419109     0.400417     106.49
 O       6.722811     0.802852    -0.065574     262.77
 H       7.105186     1.364405     0.644477      28.84
 H       6.074256    -1.240525    -0.387762      30.23
 H       6.907077    -0.924316     1.082984      28.60
55
name= lig-ACN-Water-frame_624
 C      -3.713175     1.298919    -2.366315      59.99
 H      -3.768815     0.299555    -2.953378      22.54
 C      -3.779726     2.789029    -0.573750      75.74
 H      -3.911403     2.837718     0.624973      18.19
 C      -3.366006     3.911383    -1.400531       6.01
 O      -3.141391     5.213137    -0.957198     229.44
 C      -3.206403     5.576553     0.423694      87.34
 H      -4.088110     5.301380     1.011235      27.25
 H      -3.229582     6.749647     0.069836      22.77
 H      -2.282569     5.058279     1.103137      23.28
 C      -3.313048     3.651103    -2.817072       0.20
 O      -2.849851     4.616449    -3.581968      82.84
 H      -3.065294     5.591645    -3.164427      17.73
 C      -3.318832     2.292804    -3.237816      59.36
 H      -3.286228     2.180508    -4.307990      21.30
 C      -3.986862     1.504561    -0.966262      26.14
 C      -4.243150     0.198998    -0.115891      94.09
 H      -4.809706    -0.367718    -0.816833      24.37
 O      -4.928104     0.354109     1.148553     220.88
 H      -4.236864     0.604978     1.809642      25.09
 C      -2.952603    -0.660255    -0.006193      70.60
 H      -2.437440    -0.544626    -1.017159      24.65
 C      -3.311093    -2.100550     0.631172     107.53
 O      -4.275189    -2.762332    -0.418635     182.39
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 H      -3.766284    -3.269564    -0.982008      29.19
 H      -3.965333    -1.754468     1.374366      25.43
 H      -2.325898    -2.716466     0.846861      24.42
 C       1.354531    -0.876838    -0.182869      48.34
 H       1.541128    -1.420609    -1.048609      18.33
 C       1.409327     0.774080     1.637640      51.95
 H       1.874298     1.272100     2.627991      19.31
 C       0.046673     0.478346     1.860962       7.42
 O      -0.481904     1.129764     2.932503     226.85
 C      -0.300219     2.567174     2.862313      91.06
 H       0.402728     2.902386     2.198590      25.56
 H      -1.185698     2.820801     2.551750      26.59
 H       0.011777     3.010546     4.036094      22.01
 C      -0.760228    -0.151732     0.944914      14.51
 O      -2.100290    -0.098729     1.073396     193.98
 C      -0.139234    -0.924746    -0.097312      85.29
 H      -0.699234    -1.627334    -0.671505      21.94
 C       2.084214     0.055719     0.497006      26.27
 C       3.640061     0.242772     0.022050      87.31
 H       3.521625    -0.353432    -0.883806      26.18
 O       3.793875     1.637787    -0.385026     228.21
 H       4.052316     2.181635     0.427527      25.03
 C       4.609223    -0.369770     0.942688      84.48
 H       4.603189     0.060505     2.052970      23.91
 O       4.392071    -1.800111     1.233538     236.03
 H       4.290307    -2.311404     0.291700      26.69
 C       6.257525    -0.495515     0.410328      82.90
 O       6.707002     0.845467    -0.014754     272.75
 H       7.119567     1.141868     0.871194      26.31
 H       6.199691    -1.024674    -0.643616      28.55
 H       6.870191    -0.917739     1.183427      28.88
55
name= lig-ACN-Water-frame_625
 C      -3.769817     1.225084    -2.364810      85.83
 H      -3.722399     0.154851    -2.481775      28.21
 C      -3.759650     2.936011    -0.461704      76.15
 H      -3.735069     3.197795     0.636806      17.20
 C      -3.434721     3.954608    -1.319362       9.73
 O      -3.089666     5.216650    -0.932027     222.85
 C      -3.238865     5.640909     0.455337     103.44
 H      -4.192159     5.370739     0.819492      29.68
 H      -2.900242     6.766867     0.774157      22.60
 H      -2.266119     5.127778     1.044779      23.08
 C      -3.264051     3.677097    -2.735047      -7.33
 O      -2.763121     4.670157    -3.659432      75.65
 H      -3.104955     5.671660    -3.377257      17.61
 C      -3.422464     2.341610    -3.280181      43.93
 H      -3.173812     2.037065    -4.373448      21.66
 C      -3.851198     1.561328    -1.034362     -39.75
 C      -4.232617     0.185402    -0.097822      49.14
 H      -4.981759    -0.467459    -0.620051      20.11
 O      -4.920991     0.366073     1.114154     160.58
 H      -4.395596     0.707368     1.819305      26.57
 C      -2.947312    -0.647061     0.084475      83.63
 H      -2.439787    -0.597647    -0.889872      28.79
 C      -3.338229    -2.130833     0.567086     123.88
 O      -4.302889    -2.749264    -0.312444     176.35
 H      -3.815944    -3.217954    -0.959574      29.43
 H      -3.735094    -2.161508     1.560092      27.62
 H      -2.463298    -2.831242     0.810852      27.46
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 C       1.303748    -0.860063    -0.326007      37.48
 H       1.958844    -1.343993    -0.876922      22.91
 C       1.499531     0.663213     1.616443      61.36
 H       2.231152     1.524337     2.149942      19.20
 C       0.143381     0.517488     1.898078      -9.24
 O      -0.609593     1.137389     3.000370     196.40
 C      -0.510744     2.641165     2.818272      86.68
 H       0.357025     2.705094     2.189269      25.67
 H      -1.229010     3.203260     2.534125      26.41
 H      -0.152786     3.172959     3.958089      21.30
 C      -0.648066    -0.284960     0.928641      -2.12
 O      -2.024111    -0.140074     1.096519     153.49
 C      -0.010948    -0.955705    -0.114794      69.27
 H      -0.623066    -1.437916    -0.893514      24.73
 C       2.080826     0.077821     0.494861      17.74
 C       3.549576     0.096596    -0.035309      74.50
 H       3.860136    -0.355311    -0.974561      26.16
 O       3.774900     1.554437    -0.354467     152.87
 H       4.180164     2.008844     0.488953      22.79
 C       4.809946    -0.470064     0.925699      86.17
 H       4.722124     0.276917     1.804452      25.32
 O       4.370923    -1.829812     1.232101     250.15
 H       4.224994    -2.295451     0.248675      25.24
 C       6.114062    -0.403138     0.366542     116.24
 O       6.743392     0.866329     0.055021     313.09
 H       7.182752     1.417548     0.806166      25.27
 H       6.355343    -1.195914    -0.492136      27.74
 H       6.685144    -0.956899     1.074366      29.00
55
name= lig-ACN-Water-frame_626
 C      -3.717067     1.325236    -2.383862      22.86
 H      -3.847165     0.485120    -2.960456      21.02
 C      -3.737587     2.881189    -0.368909      71.00
 H      -3.884372     3.021148     0.664152      20.55
 C      -3.435512     3.972321    -1.335371     -16.11
 O      -3.048753     5.315088    -0.928755     214.75
 C      -3.205175     5.628216     0.531074     104.79
 H      -4.217242     5.557273     0.829286      25.44
 H      -3.021202     6.768366     0.392338      22.20
 H      -2.646318     4.880954     1.323902      23.61
 C      -3.166538     3.687751    -2.777020       4.55
 O      -2.732712     4.669750    -3.682526     124.28
 H      -3.133371     5.583287    -3.326646      22.60
 C      -3.524609     2.392819    -3.213648      44.30
 H      -3.173691     2.330125    -4.364000      21.55
 C      -3.858565     1.543262    -0.866474      22.69
 C      -4.119721     0.330323    -0.125412      79.17
 H      -4.673756    -0.306938    -0.917423      25.03
 O      -4.954460     0.437724     1.131004     171.59
 H      -4.261065     0.643256     1.851515      23.32
 C      -2.897025    -0.781971     0.165687      89.02
 H      -2.416786    -1.012586    -0.729976      27.47
 C      -3.337414    -2.139224     0.565876     130.46
 O      -4.336944    -2.708070    -0.282039     183.13
 H      -3.823905    -3.393521    -0.941483      24.42
 H      -3.679655    -2.167584     1.566605      28.57
 H      -2.384560    -2.687810     0.290796      25.58
 C       1.404251    -0.797821    -0.447597      49.23
 H       1.606779    -1.335525    -1.255200      26.48
 C       1.617415     0.612276     1.573574      22.29
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 H       2.342241     1.473407     2.135054      18.89
 C       0.159071     0.509264     1.904070     -19.04
 O      -0.664523     1.185789     2.951422     148.69
 C      -0.640786     2.688957     2.813959      86.94
 H       0.129499     3.196550     2.130383      24.51
 H      -1.535764     2.794599     2.494042      26.57
 H      -0.504114     3.070132     4.049280      21.16
 C      -0.575482    -0.310545     0.981257      -1.15
 O      -1.972890    -0.170001     1.115311      94.87
 C      -0.026123    -1.021033    -0.168306      68.53
 H      -0.601628    -1.679330    -0.915890      21.54
 C       2.186852    -0.103532     0.441734      25.46
 C       3.578712     0.131293    -0.014721      99.47
 H       3.368646    -0.439286    -0.922283      24.51
 O       3.791834     1.490020    -0.334197     224.55
 H       4.173037     1.990753     0.452337      24.35
 C       4.627624    -0.477468     0.897306      93.64
 H       4.714301    -0.127539     1.945411      26.42
 O       4.375954    -1.857251     1.230085     259.96
 H       4.519629    -2.431594     0.409118      29.55
 C       6.236944    -0.404061     0.304302      91.68
 O       6.743689     0.904928     0.040949     259.40
 H       7.180946     1.168683     0.873840      27.13
 H       6.021142    -0.812104    -0.764364      28.14
 H       6.867977    -0.846790     1.016874      29.15
55
name= lig-ACN-Water-frame_627
 C      -3.704743     1.457949    -2.260846      60.47
 H      -3.919346     0.501333    -2.561321      26.99
 C      -3.692999     2.863981    -0.438457      80.83
 H      -3.937525     3.068943     0.543900      20.15
 C      -3.290431     3.984184    -1.292292      13.35
 O      -3.054777     5.277962    -0.876930     233.49
 C      -3.253508     5.630749     0.491976     115.48
 H      -4.275632     5.631695     0.794869      26.94
 H      -2.673390     6.583518     0.690537      22.13
 H      -2.520191     4.976098     1.177634      22.09
 C      -3.163825     3.786313    -2.680577      29.62
 O      -2.752416     4.652507    -3.638023     177.53
 H      -2.884287     5.538517    -3.270061      25.16
 C      -3.457273     2.520008    -3.214777      54.77
 H      -3.737241     2.153575    -4.312106      21.49
 C      -3.798471     1.604030    -0.955061      37.61
 C      -4.027480     0.230625    -0.022941      74.77
 H      -4.804954    -0.454853    -0.634672      20.91
 O      -4.930426     0.529609     1.082802     188.71
 H      -4.454098     0.642533     2.045461      19.43
 C      -2.878318    -0.690693     0.104446      81.42
 H      -2.437446    -0.610541    -0.801626      24.96
 C      -3.258183    -2.228181     0.650490     105.05
 O      -4.399782    -2.653111    -0.318892     204.15
 H      -3.889893    -3.368377    -1.046037      20.22
 H      -3.630458    -2.228310     1.677097      25.85
 H      -2.386233    -2.931774     0.774089      25.34
 C       1.300415    -0.886408    -0.523614      20.98
 H       1.752767    -0.993818    -1.424538      20.87
 C       1.574065     0.559656     1.560384      61.02
 H       2.234743     1.071155     2.457526      19.03
 C       0.233017     0.490403     1.824343      21.09
 O      -0.495883     1.207010     2.760848     230.56
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 C      -0.843501     2.657041     2.836394      92.34
 H      -0.079215     3.277030     2.178419      22.90
 H      -1.746801     2.949291     2.541779      24.92
 H      -0.813081     3.151695     4.041959      21.93
 C      -0.567268    -0.311119     0.956661      12.79
 O      -1.929905    -0.244192     1.156946     129.33
 C       0.013983    -0.981507    -0.123402      52.63
 H      -0.695037    -1.719483    -0.655045      20.89
 C       2.175835    -0.171747     0.466202      21.83
 C       3.637105     0.100043    -0.042796      81.73
 H       4.063526    -0.260229    -0.978432      23.64
 O       3.848305     1.533297    -0.344290     190.73
 H       4.053698     2.037389     0.467112      26.27
 C       4.653430    -0.493624     0.953269      94.46
 H       4.384795     0.141354     1.782482      26.24
 O       4.391544    -1.927306     1.199190     276.12
 H       4.457093    -2.323017     0.367266      30.97
 C       6.188859    -0.406743     0.235405      84.34
 O       6.745073     0.963580    -0.010539     226.43
 H       6.988894     1.432762     0.821839      27.42
 H       6.264289    -0.913082    -0.835114      28.12
 H       6.829812    -1.146315     0.646640      29.98
55
name= lig-ACN-Water-frame_628
 C      -3.716831     1.413237    -2.367618      44.12
 H      -3.787041     0.455037    -2.854989      25.47
 C      -3.627107     3.000984    -0.386171      84.93
 H      -3.790152     3.182937     0.669897      18.57
 C      -3.161790     3.962201    -1.230526      23.39
 O      -3.057169     5.263066    -0.840110     248.44
 C      -3.205903     5.623905     0.517264     100.32
 H      -4.291534     5.701058     0.782397      26.02
 H      -2.804635     6.584392     0.629597      24.87
 H      -2.862605     4.744410     1.196312      28.02
 C      -3.154897     3.749845    -2.655952       6.59
 O      -2.746383     4.758840    -3.587045     154.62
 H      -3.109769     5.603659    -3.305070      22.09
 C      -3.445644     2.514902    -3.146244      65.20
 H      -3.441857     2.603402    -4.294402      20.78
 C      -3.705913     1.564966    -0.849114     -44.00
 C      -4.129085     0.233418    -0.010608      74.93
 H      -4.706845    -0.534904    -0.768409      22.43
 O      -4.902451     0.616620     1.086500     248.04
 H      -4.300017     0.656065     1.951711      20.65
 C      -2.777943    -0.726868     0.182191      87.28
 H      -2.380560    -0.803621    -0.746215      27.53
 C      -3.303901    -2.183047     0.575314     128.76
 O      -4.347348    -2.604528    -0.255386     210.78
 H      -3.902789    -3.190869    -1.032090      24.26
 H      -3.817788    -1.920279     1.517805      26.13
 H      -2.572514    -2.959835     0.615165      28.07
 C       1.350481    -0.849124    -0.453083      48.88
 H       1.610230    -1.429708    -1.344309      21.69
 C       1.649886     0.416096     1.545902      40.23
 H       2.376463     0.991723     2.251710      19.71
 C       0.220152     0.561151     1.663302       1.65
 O      -0.338128     1.246630     2.711014     210.42
 C      -0.971077     2.617243     2.774636      76.78
 H      -0.193802     3.415834     2.294351      20.76
 H      -1.937060     2.610750     2.443028      21.66
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 H      -0.823787     2.579672     4.029634      19.15
 C      -0.594978    -0.302568     0.879855      16.44
 O      -1.918747    -0.289779     1.210650     196.00
 C      -0.077551    -1.052548    -0.139500      51.05
 H      -0.705416    -1.570811    -0.918136      19.35
 C       2.181328    -0.123125     0.348148      34.02
 C       3.652635     0.073151    -0.078368      64.99
 H       3.536917    -0.475664    -1.035920      25.60
 O       3.891616     1.591709    -0.346892     170.68
 H       3.997096     2.063337     0.514284      24.44
 C       4.826870    -0.506035     0.936545      89.66
 H       5.057156    -0.170591     1.876392      26.94
 O       4.419633    -1.915936     1.165310     278.73
 H       4.257217    -2.288398     0.328702      30.87
 C       6.106246    -0.361096     0.209200      95.83
 O       6.720471     0.959559    -0.042822     252.06
 H       6.846823     1.341331     0.908849      27.56
 H       5.760731    -0.754877    -0.856016      27.50
 H       6.823430    -0.796878     0.859208      29.02
55
name= lig-ACN-Water-frame_629
 C      -3.668011     1.343922    -2.310186      28.67
 H      -3.838264     0.355601    -2.829051      21.07
 C      -3.534347     2.810114    -0.284491      71.13
 H      -3.745578     2.983769     0.837920      20.67
 C      -3.144484     3.995157    -1.217908     -21.59
 O      -2.993791     5.324442    -0.842279     181.89
 C      -3.220219     5.601300     0.612821     126.62
 H      -4.341023     5.767314     0.751438      24.66
 H      -2.669394     6.425587     0.662309      27.10
 H      -2.709132     5.023712     1.408911      26.09
 C      -3.047652     3.815152    -2.657213       4.09
 O      -2.768818     4.853124    -3.495252     182.39
 H      -3.148035     5.698257    -3.188252      19.73
 C      -3.424032     2.478667    -3.189571      30.31
 H      -3.137254     2.226369    -4.208860      23.70
 C      -3.708032     1.547909    -0.903649      50.31
 C      -4.049866     0.350413    -0.123214      53.98
 H      -4.948970    -0.149480    -0.800020      23.29
 O      -4.909552     0.657081     1.138615     145.95
 H      -4.370398     0.604680     1.990890      22.26
 C      -2.884421    -0.762636     0.204197      83.17
 H      -2.272337    -0.760409    -0.655931      28.10
 C      -3.359667    -2.053488     0.637982     133.31
 O      -4.370193    -2.613116    -0.273141     225.36
 H      -3.872373    -3.139417    -0.865879      30.09
 H      -3.649899    -2.211484     1.698405      27.18
 H      -2.478473    -2.636144     0.672121      28.46
 C       1.287654    -0.931664    -0.482409      27.65
 H       1.841519    -1.624539    -1.224868      21.62
 C       1.684810     0.430228     1.495518      47.39
 H       2.252918     1.030765     2.202853      21.00
 C       0.292335     0.606127     1.543624       2.45
 O      -0.206068     1.277719     2.761558     199.58
 C      -0.967472     2.479802     2.732705      91.12
 H      -0.600345     3.510835     2.220941      23.17
 H      -1.846519     2.399366     2.152636      25.82
 H      -1.405492     2.924792     3.812727      22.62
 C      -0.608221    -0.244163     0.816162      -2.11
 O      -1.941903    -0.291807     1.258174     140.28
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 C      -0.037335    -1.089394    -0.266959      52.60
 H      -0.546815    -1.828657    -0.889338      22.78
 C       2.242417    -0.082648     0.325771      28.86
 C       3.676412     0.179498     0.004813     101.49
 H       3.999722    -0.251689    -0.966509      24.99
 O       3.884198     1.529760    -0.392267     207.66
 H       4.042792     2.107572     0.425181      26.20
 C       4.746126    -0.475529     0.847626     107.19
 H       4.585853     0.124097     1.660755      30.00
 O       4.477551    -1.839022     1.150275     297.87
 H       4.595242    -2.286520     0.317706      30.46
 C       6.209542    -0.362630     0.127803      98.85
 O       6.642828     0.972766    -0.040066     248.44
 H       7.210745     1.314909     0.753020      26.67
 H       6.364771    -0.814736    -1.002337      27.92
 H       6.874898    -1.153255     0.493575      30.86
55
name= lig-ACN-Water-frame_630
 C      -3.575624     1.427822    -2.324063      57.88
 H      -3.838684     0.326365    -2.598019      22.64
 C      -3.354009     2.812168    -0.393654      75.62
 H      -3.528238     2.791054     0.802774      19.29
 C      -3.219849     3.909286    -1.122850      -4.64
 O      -2.929958     5.295657    -0.748121     230.94
 C      -3.163203     5.669520     0.643144     117.08
 H      -4.289391     5.649007     0.942429      25.45
 H      -2.770332     6.508394     0.948784      27.21
 H      -2.844000     4.794697     1.112506      27.12
 C      -3.041238     3.741044    -2.605097      -8.43
 O      -2.771601     4.899096    -3.435764     114.87
 H      -3.054437     5.718911    -2.987493      23.33
 C      -3.255369     2.441213    -3.201427      65.45
 H      -3.359550     2.226679    -4.202886      24.08
 C      -3.713282     1.572195    -0.958587      43.34
 C      -4.087435     0.391278    -0.022828      90.03
 H      -4.696333    -0.482763    -0.714700      23.95
 O      -4.899453     0.663818     1.093184     205.91
 H      -4.320031     0.732402     1.873935      23.60
 C      -3.005488    -0.555654     0.171238      76.05
 H      -2.666525    -0.878302    -0.837688      28.64
 C      -3.406327    -2.118113     0.762700     103.14
 O      -4.420441    -2.636418    -0.295500     151.36
 H      -3.961029    -3.277978    -0.752194      30.42
 H      -3.944024    -1.989178     1.731217      25.76
 H      -2.611633    -2.715281     0.712375      28.75
 C       1.462598    -0.996644    -0.524383      61.30
 H       1.971853    -1.543164    -1.482593      17.23
 C       1.654310     0.632189     1.386291      59.03
 H       2.243141     1.005522     2.115332      23.17
 C       0.272339     0.612028     1.623476       6.62
 O      -0.043429     1.270513     2.811155     216.19
 C      -1.051725     2.410327     2.583881      65.51
 H      -0.208052     3.134299     2.212304      23.32
 H      -1.834069     2.117922     1.922930      24.83
 H      -1.404535     2.559626     3.695150      22.07
 C      -0.593361    -0.200659     0.733269      13.56
 O      -1.936179    -0.267278     1.225856     143.18
 C      -0.035190    -1.022546    -0.260416     104.57
 H      -0.618952    -1.854918    -0.517459      23.74
 C       2.182286    -0.180462     0.315989      39.44
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 C       3.701198     0.135455    -0.198707      56.36
 H       3.712017    -0.458383    -1.134036      23.54
 O       3.855332     1.553881    -0.429326     196.89
 H       3.829047     2.108789     0.449557      25.13
 C       4.774661    -0.369720     0.840934     100.42
 H       5.017619     0.034334     1.730999      28.79
 O       4.523454    -1.756367     1.165174     243.57
 H       4.346744    -2.206416     0.266125      27.86
 C       6.280787    -0.421848     0.050616      82.62
 O       6.676562     1.049934    -0.011127     204.46
 H       7.220847     1.177994     0.781506      30.90
 H       5.923441    -0.789760    -1.041587      29.74
 H       6.946452    -0.819317     0.818585      29.54
55
name= lig-ACN-Water-frame_631
 C      -3.536233     1.371238    -2.368834      34.66
 H      -3.710126     0.486086    -3.115921      19.57
 C      -3.313250     2.832101    -0.339438      64.09
 H      -3.208688     3.104061     0.846761      19.39
 C      -3.132586     4.004577    -1.209891       6.46
 O      -2.895028     5.220236    -0.681496     227.86
 C      -3.129050     5.569163     0.709819     112.39
 H      -4.257783     5.781685     0.748848      23.82
 H      -2.546797     6.438450     0.655021      25.62
 H      -2.735630     5.040944     1.494350      29.69
 C      -3.078344     3.782946    -2.586695       7.21
 O      -2.764046     4.808885    -3.350720     115.18
 H      -3.281183     5.670628    -3.092049      23.97
 C      -3.094092     2.511622    -3.192386      43.76
 H      -3.061201     2.669796    -4.215371      20.57
 C      -3.666494     1.561323    -0.896942      11.79
 C      -4.159959     0.366434    -0.057968      63.91
 H      -4.978554    -0.203708    -0.812169      20.96
 O      -4.938512     0.719321     1.095471     203.46
 H      -4.411517     0.930877     1.920919      24.01
 C      -2.952739    -0.726887     0.278048      82.88
 H      -2.404324    -0.628831    -0.723155      23.04
 C      -3.569063    -2.027375     0.688716     135.61
 O      -4.463710    -2.636531    -0.213424     272.74
 H      -3.884836    -3.229063    -0.757995      26.29
 H      -4.146892    -1.963799     1.629695      26.39
 H      -2.839819    -2.596632     1.011202      29.78
 C       1.383384    -1.002553    -0.490852      62.11
 H       1.677288    -1.662841    -1.487236      21.30
 C       1.660436     0.699993     1.208684      72.60
 H       2.209530     1.335548     1.713680      23.50
 C       0.328987     0.578787     1.660087       8.40
 O      -0.033532     1.258578     2.847368     272.25
 C      -0.967827     2.294815     2.498570      72.50
 H      -0.721080     3.347749     2.120559      22.71
 H      -1.694601     1.920191     1.678710      21.44
 H      -1.597971     2.570246     3.370483      20.85
 C      -0.548461    -0.132801     0.800182      19.06
 O      -1.913515    -0.195062     1.079396     204.91
 C       0.076649    -1.002660    -0.203768      27.53
 H      -0.541237    -1.490307    -0.900991      20.51
 C       2.288320    -0.161964     0.249197      43.52
 C       3.623335     0.095975    -0.207253      75.75
 H       3.828915    -0.360488    -1.178608      26.16
 O       3.776048     1.575483    -0.507653      99.64
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 H       3.837056     1.998309     0.441335      24.83
 C       4.954423    -0.385037     0.738658      97.17
 H       4.816467     0.327711     1.472168      29.41
 O       4.529246    -1.688700     1.214992     244.92
 H       4.284939    -2.260511     0.306315      25.02
 C       6.198927    -0.261680     0.117327     112.67
 O       6.786138     1.075096    -0.014933     251.46
 H       7.095113     1.341075     0.880208      29.31
 H       6.458650    -0.772633    -0.973427      26.11
 H       6.937816    -1.044540     0.482987      28.87
55
name= lig-ACN-Water-frame_632
 C      -3.454058     1.430628    -2.358013      56.91
 H      -3.654776     0.349392    -2.656178      23.66
 C      -3.362702     2.818174    -0.354123      90.40
 H      -3.404773     2.891608     0.813682      18.11
 C      -3.055502     3.889990    -1.106383      24.16
 O      -2.819189     5.179209    -0.662327     260.80
 C      -3.076891     5.566251     0.741701     107.80
 H      -4.164766     5.712790     0.969169      26.65
 H      -2.613833     6.582971     0.966502      25.46
 H      -2.748464     4.892827     1.383243      34.83
 C      -3.056252     3.782981    -2.506070      16.77
 O      -2.739259     4.896760    -3.428521     132.50
 H      -3.199003     5.801885    -3.009971      19.16
 C      -3.072478     2.545841    -3.109835      69.95
 H      -2.672217     2.187882    -4.029878      24.90
 C      -3.577213     1.558464    -0.981306       9.99
 C      -4.091375     0.346475    -0.107109      46.03
 H      -4.921817    -0.319354    -0.706333      21.61
 O      -5.016125     0.803119     1.119842      88.41
 H      -4.381874     0.777641     1.955799      21.62
 C      -2.927032    -0.744639     0.102515      71.87
 H      -2.595549    -1.405298    -0.829849      20.48
 C      -3.656330    -1.990305     0.827971     113.20
 O      -4.523138    -2.643364    -0.190261     181.41
 H      -3.926424    -3.225656    -0.915975      24.20
 H      -4.304613    -1.518997     1.546415      26.27
 H      -3.029801    -2.661070     1.113516      29.13
 C       1.385250    -1.000524    -0.442459      36.38
 H       1.861889    -1.765503    -1.250659      22.11
 C       1.738124     0.705416     1.151498      71.65
 H       2.189283     1.579400     1.495568      23.10
 C       0.442243     0.558665     1.636065       4.08
 O      -0.036109     1.262922     2.826951     241.81
 C      -1.012694     2.275812     2.454365      75.01
 H      -0.300928     3.074161     2.111056      22.81
 H      -1.646564     1.859535     1.523034      16.84
 H      -1.681335     2.436098     3.232274      21.09
 C      -0.532163    -0.243373     0.843264      23.29
 O      -1.911110    -0.085807     1.070585     154.29
 C      -0.031834    -0.954975    -0.166103      62.15
 H      -0.662762    -1.365916    -0.938864      21.09
 C       2.267311    -0.103423     0.160837      35.68
 C       3.759663     0.143497    -0.230466     114.78
 H       3.891984    -0.391931    -1.172618      27.07
 O       3.706896     1.554923    -0.535182     151.22
 H       3.935661     2.152909     0.242295      20.71
 C       4.716581    -0.304796     0.705456     101.00
 H       4.843489     0.190095     1.641171      27.58
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 O       4.568520    -1.642703     1.256941     236.93
 H       4.791796    -2.350850     0.485539      27.20
 C       6.417866    -0.216019     0.031419      63.75
 O       6.909851     1.121416     0.007726     211.65
 H       7.111538     1.485082     0.949777      25.04
 H       6.044033    -0.436345    -1.080140      25.19
 H       6.953950    -0.792957     0.827112      27.56
55
name= lig-ACN-Water-frame_633
 C      -3.363329     1.395679    -2.303637      67.71
 H      -3.282076     0.481495    -2.899247      24.05
 C      -3.434042     2.709693    -0.270893      78.14
 H      -3.837451     2.725423     0.742697      22.22
 C      -3.028372     3.918810    -1.047485      -7.34
 O      -2.734461     5.217064    -0.606495     217.89
 C      -3.024613     5.524559     0.756399     106.21
 H      -4.089846     5.466401     0.861031      26.79
 H      -2.435796     6.522438     1.055727      23.99
 H      -2.608620     4.858958     1.319659      33.19
 C      -2.914931     3.840726    -2.568986     -17.93
 O      -2.740396     4.991838    -3.451981      97.18
 H      -2.883104     5.838324    -2.865764      25.06
 C      -3.050361     2.478455    -3.108730      33.66
 H      -2.901599     2.547020    -4.249658      19.49
 C      -3.609812     1.507246    -0.883735      37.39
 C      -4.027729     0.359830    -0.153172      61.43
 H      -4.777707    -0.219917    -0.880403      23.10
 O      -4.933045     0.816936     1.035223     106.42
 H      -4.517936     0.624288     1.947271      21.71
 C      -3.015597    -0.725113     0.118018      63.94
 H      -2.477531    -0.775767    -0.996219      23.55
 C      -3.701793    -1.952290     0.923554     115.00
 O      -4.576943    -2.604636    -0.157733     146.72
 H      -3.916034    -3.424617    -0.566765      22.38
 H      -4.411481    -1.677740     1.652087      27.79
 H      -3.106215    -2.496680     1.457653      30.77
 C       1.384561    -1.042078    -0.458126      25.29
 H       1.733575    -1.785587    -1.279435      21.22
 C       1.729184     0.755623     1.214117      44.04
 H       2.422683     1.443300     1.942280      21.00
 C       0.391992     0.546212     1.666575      18.33
 O      -0.005434     1.198126     2.749148     220.84
 C      -1.005256     2.317643     2.398213      87.57
 H      -0.547289     3.266505     2.201600      26.57
 H      -1.765293     2.169430     1.389736      22.06
 H      -1.546047     2.479386     3.197687      27.18
 C      -0.549278    -0.287525     0.929291      -7.12
 O      -1.945491    -0.055114     1.042067      66.12
 C      -0.031653    -1.012945    -0.281792      77.39
 H      -0.695744    -1.823402    -0.691109      22.06
 C       2.242224    -0.093255     0.126923      25.48
 C       3.631520     0.149489    -0.347929      83.81
 H       3.961874    -0.364859    -1.234671      26.17
 O       3.756828     1.643536    -0.539851     206.13
 H       3.884177     1.975247     0.358845      24.80
 C       4.873103    -0.246710     0.843624      68.95
 H       4.682157     0.523230     1.663642      24.88
 O       4.608928    -1.626652     1.241961     256.58
 H       4.874752    -2.137847     0.509599      31.40
 C       6.351590    -0.149124     0.068974      84.06
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 O       7.042160     1.209158     0.015721     190.65
 H       7.266836     1.362999     1.031388      25.25
 H       6.580817    -0.704585    -0.979456      25.05
 H       7.111457    -0.910858     0.488049      27.15
55
name= lig-ACN-Water-frame_634
 C      -3.236391     1.350862    -2.330742      47.84
 H      -3.354859     0.380266    -2.735591      26.78
 C      -3.480701     2.896386    -0.261167      70.25
 H      -3.766329     3.142676     0.677634      20.82
 C      -3.005684     3.947225    -1.116691      -2.26
 O      -2.656753     5.207866    -0.596096     199.36
 C      -2.958485     5.421546     0.826934     130.17
 H      -3.968748     5.543197     1.016819      25.87
 H      -2.607247     6.600629     0.858281      22.82
 H      -2.568460     4.862455     1.476632      33.29
 C      -2.804823     3.852350    -2.524126      31.88
 O      -2.735839     4.953152    -3.358060     191.34
 H      -2.975839     5.773822    -2.977690      24.16
 C      -3.009642     2.622972    -3.131064      27.07
 H      -3.272618     2.350732    -4.254766      24.83
 C      -3.561691     1.533734    -0.951812     -32.85
 C      -4.151058     0.287731    -0.102935      89.74
 H      -4.860852    -0.355882    -0.769638      26.82
 O      -4.813723     0.775753     0.926719     195.70
 H      -4.448884     0.564489     1.776384      24.17
 C      -3.023410    -0.675015     0.328386      88.23
 H      -2.508211    -1.216533    -0.703087      25.74
 C      -3.744917    -1.894718     0.847276     134.50
 O      -4.560576    -2.601726    -0.044192     185.33
 H      -3.987896    -3.234365    -0.623548      26.92
 H      -4.363871    -1.510534     1.596796      27.21
 H      -3.049601    -2.546480     1.103234      30.00
 C       1.334655    -1.028906    -0.538510      59.48
 H       1.789507    -1.615416    -1.332229      23.17
 C       1.652233     0.601367     1.231806      53.65
 H       2.373207     1.114746     2.116731      20.31
 C       0.329950     0.494653     1.570186      11.95
 O      -0.104029     1.269028     2.726025     211.51
 C      -0.945488     2.399512     2.446433     102.25
 H      -0.362152     3.220835     2.260858      26.86
 H      -1.603335     1.943848     1.425758      22.25
 H      -1.597154     2.469159     3.169919      27.46
 C      -0.574433    -0.315513     0.751894      13.10
 O      -1.975859    -0.085128     1.068526     158.57
 C       0.004452    -1.136566    -0.159833      60.24
 H      -0.530239    -1.906538    -0.801737      23.29
 C       2.181460    -0.077879     0.179982      30.43
 C       3.666132     0.229201    -0.249251      80.09
 H       3.759746    -0.191068    -1.249724      22.91
 O       3.837731     1.701787    -0.527426     218.04
 H       3.942806     2.257376     0.277266      24.57
 C       4.981986    -0.224399     0.724803      81.42
 H       4.926523     0.404080     1.739583      22.91
 O       4.697419    -1.564171     1.220447     275.02
 H       4.519882    -2.146826     0.472936      29.24
 C       6.357743    -0.059343     0.186358      81.77
 O       7.086192     1.183638     0.013811     250.93
 H       7.455102     1.551021     0.905592      27.25
 H       5.990480    -0.214090    -0.907684      26.94
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 H       6.920945    -0.779772     0.878553      26.89
55
name= lig-ACN-Water-frame_635
 C      -3.169709     1.498021    -2.319303      67.36
 H      -3.314282     0.600412    -2.802586      24.54
 C      -3.503990     2.927234    -0.460308      91.08
 H      -3.621288     2.983509     0.513280      22.67
 C      -2.943131     4.000334    -1.083726      19.04
 O      -2.613054     5.171781    -0.563455     236.14
 C      -2.908054     5.449097     0.850748      91.54
 H      -3.870471     5.207498     1.017487      28.82
 H      -2.432646     6.505872     1.241980      22.59
 H      -2.371521     4.836424     1.329793      36.22
 C      -2.827298     3.813515    -2.527757       9.76
 O      -2.686961     4.925340    -3.291191      86.53
 H      -3.247946     5.655346    -2.998443      20.81
 C      -3.010518     2.550908    -3.113872      52.79
 H      -2.859671     2.677079    -4.299802      20.53
 C      -3.535947     1.643589    -0.967735      21.77
 C      -4.017965     0.323125    -0.251670      71.10
 H      -4.711732    -0.352594    -0.853694      24.42
 O      -4.884701     0.803512     1.008678     103.25
 H      -4.419810     0.565832     1.865403      22.98
 C      -3.006685    -0.714612     0.242528      68.63
 H      -2.450555    -1.156956    -0.824237      20.35
 C      -3.688009    -1.954416     0.993465     113.94
 O      -4.591785    -2.625212    -0.034152     231.49
 H      -4.082862    -2.932157    -0.688641      32.86
 H      -4.326401    -1.890266     1.831366      25.84
 H      -2.933706    -2.526029     1.386008      28.52
 C       1.419958    -0.939435    -0.576078      51.99
 H       1.714079    -1.499194    -1.384348      23.57
 C       1.587210     0.421438     1.342777      21.89
 H       2.290097     1.244673     1.972454      17.33
 C       0.167734     0.544151     1.541732      11.42
 O      -0.173562     1.238189     2.688212     246.60
 C      -0.931594     2.461164     2.460138      97.59
 H      -0.285788     3.224275     2.363532      26.33
 H      -1.596731     2.673445     1.349033      19.51
 H      -1.520555     2.685681     3.210047      26.49
 C      -0.666043    -0.233311     0.716427       3.29
 O      -1.971417    -0.154296     1.158168     148.88
 C      -0.010321    -1.316034    -0.135669      34.01
 H      -0.722995    -1.890153    -0.790738      18.68
 C       2.262338    -0.121856     0.170813      27.47
 C       3.762118     0.351643    -0.141268      99.47
 H       4.027725    -0.234201    -1.039462      23.62
 O       3.891982     1.715167    -0.500048     238.80
 H       4.104594     2.203516     0.365438      23.74
 C       4.805689    -0.116906     0.754058      84.69
 H       4.792106     0.486953     1.786138      22.90
 O       4.819445    -1.527840     1.161716     244.71
 H       4.298201    -2.125946     0.430433      25.37
 C       6.381825    -0.052467     0.106860      89.00
 O       7.089282     1.193977     0.010330     216.70
 H       7.247788     1.337457     1.002711      27.81
 H       6.614807    -0.653650    -0.866480      28.22
 H       7.047807    -0.798289     0.683875      29.21
55
name= lig-ACN-Water-frame_636
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 C      -3.229729     1.423660    -2.371032      54.28
 H      -3.049716     0.467332    -2.775341      23.31
 C      -3.496355     2.886702    -0.361237      64.93
 H      -3.897684     2.923478     0.618008      21.34
 C      -2.925204     3.983846    -1.139447       1.33
 O      -2.561758     5.289326    -0.531918     211.45
 C      -2.814527     5.357140     0.876590     117.93
 H      -3.799837     5.336098     1.170190      28.03
 H      -2.623483     6.542259     0.959774      23.86
 H      -2.262517     4.856313     1.493356      36.52
 C      -2.912212     3.897769    -2.509859      15.07
 O      -2.605058     4.970643    -3.329933     173.63
 H      -3.057895     5.896133    -3.044831      17.35
 C      -2.938581     2.649653    -3.173949      44.71
 H      -2.635663     2.361599    -4.276433      23.64
 C      -3.523956     1.577328    -1.019509      11.40
 C      -3.960398     0.458269    -0.190235      84.80
 H      -4.621500     0.062287    -0.895902      26.38
 O      -4.937895     0.810630     0.999334     116.39
 H      -4.504794     0.442121     1.880144      21.67
 C      -3.011813    -0.778788     0.196117      69.33
 H      -2.308237    -1.079450    -0.805557      21.65
 C      -3.635551    -2.066946     1.003125     115.49
 O      -4.589353    -2.639827     0.017702     212.49
 H      -4.016528    -3.200270    -0.613137      27.13
 H      -4.269573    -1.589396     1.720016      26.62
 H      -2.865535    -2.755247     1.265039      28.15
 C       1.370346    -1.000568    -0.566578      17.48
 H       1.746012    -1.361139    -1.428921      21.81
 C       1.598332     0.445496     1.379217      43.78
 H       2.121859     1.077046     2.282356      19.24
 C       0.250199     0.527765     1.519759      15.36
 O      -0.327370     1.199321     2.642674     204.09
 C      -0.876925     2.630636     2.474151      78.03
 H      -0.127300     3.284803     2.519629      25.57
 H      -1.639534     2.485396     1.427010      17.56
 H      -1.498740     2.693640     3.296644      24.34
 C      -0.666055    -0.335274     0.762866       5.87
 O      -2.021408    -0.267176     1.158406     179.71
 C       0.026118    -1.134506    -0.171997      37.34
 H      -0.361286    -2.028518    -0.656390      22.85
 C       2.256536    -0.122862     0.268212      24.27
 C       3.704744     0.270034    -0.206010      71.34
 H       3.912316    -0.132349    -1.234796      28.12
 O       3.929078     1.750460    -0.456581     161.42
 H       4.037292     2.281152     0.449618      24.14
 C       4.930848    -0.108328     0.850395      82.25
 H       4.853651     0.545468     1.848224      24.91
 O       4.851558    -1.509620     1.111139     229.86
 H       4.499004    -1.888564     0.238825      29.30
 C       6.372345    -0.144495     0.053811      86.36
 O       7.060845     1.229989    -0.010578     157.71
 H       7.280463     1.440471     0.897950      29.68
 H       6.232002    -0.578883    -0.948905      28.02
 H       6.841606    -0.668900     0.923454      28.13
55
name= lig-ACN-Water-frame_637
 C      -3.242203     1.451513    -2.451068      56.97
 H      -3.228015     0.446317    -2.915773      21.77
 C      -3.392511     2.886012    -0.333085      73.35
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 H      -3.739654     3.073442     0.744630      18.48
 C      -3.011932     4.042743    -1.042816       6.72
 O      -2.573426     5.239989    -0.580402     217.47
 C      -2.752331     5.414706     0.925614      77.31
 H      -3.729584     5.043747     1.090470      28.79
 H      -2.440678     6.464513     1.238353      23.07
 H      -2.103661     4.755750     1.355861      31.83
 C      -2.916001     3.966602    -2.590711     -23.21
 O      -2.510821     5.062943    -3.413596      17.55
 H      -2.895960     5.995497    -2.981905      21.52
 C      -2.965791     2.613772    -3.134551      52.51
 H      -2.831781     2.682105    -4.261633      21.96
 C      -3.479189     1.628974    -0.984061      -1.13
 C      -4.119584     0.309518    -0.062137      76.76
 H      -4.713501    -0.339068    -0.590161      27.86
 O      -4.899377     0.807602     0.935242     239.32
 H      -4.467854     0.696014     1.869016      22.25
 C      -2.977771    -0.803808     0.249093      91.20
 H      -2.739965    -1.212215    -0.905521      22.61
 C      -3.628329    -2.015381     0.773743     124.31
 O      -4.584125    -2.743928     0.067923     165.50
 H      -4.087935    -3.573607    -0.510736      23.83
 H      -4.134716    -1.949109     1.784522      26.57
 H      -2.836272    -2.691982     1.163325      27.81
 C       1.446095    -0.924862    -0.453888      37.63
 H       1.726736    -1.563926    -1.233762      20.47
 C       1.688628     0.588950     1.410560      47.40
 H       2.464726     0.989032     2.166441      18.42
 C       0.196393     0.492492     1.611944      12.61
 O      -0.476724     1.205031     2.606430     261.87
 C      -0.829520     2.580408     2.514994      83.19
 H       0.021735     3.330686     2.492321      23.03
 H      -1.442503     2.930487     1.418866      17.20
 H      -1.499872     2.899809     3.267899      22.95
 C      -0.583416    -0.396064     0.867236       9.92
 O      -1.945531    -0.386117     1.109933     250.80
 C      -0.023073    -1.029526    -0.275304      85.98
 H      -0.666629    -1.683621    -0.824473      19.98
 C       2.225858    -0.123799     0.291200      33.42
 C       3.705311     0.250808    -0.131784      71.94
 H       3.790790    -0.328650    -1.102682      25.91
 O       3.893618     1.731646    -0.436889     162.91
 H       4.052217     2.141474     0.541158      22.69
 C       5.002008    -0.181624     0.693668     109.99
 H       5.065533     0.333641     1.768692      24.60
 O       4.807625    -1.561510     1.103370     289.22
 H       4.923648    -2.127836     0.400414      32.74
 C       6.363294    -0.041817     0.175630     124.31
 O       6.994370     1.188946    -0.090261     240.19
 H       7.181225     1.544872     0.787036      29.68
 H       6.187717    -0.380290    -0.856462      28.20
 H       7.090114    -0.808186     0.260371      30.21
55
name= lig-ACN-Water-frame_638
 C      -3.292625     1.546433    -2.297785      43.08
 H      -3.614269     0.685294    -2.974599      21.25
 C      -3.306054     2.865562    -0.399009      51.75
 H      -3.227805     2.795873     0.804347      15.05
 C      -3.048463     4.067637    -1.201253       5.22
 O      -2.620557     5.252952    -0.535989     264.26
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 C      -2.684208     5.402094     0.875333      98.68
 H      -3.676948     5.306439     1.429916      24.26
 H      -2.445128     6.405250     1.049705      21.39
 H      -1.898685     4.827075     1.388632      28.76
 C      -2.854829     3.972778    -2.544773      30.64
 O      -2.439700     5.029020    -3.409690     132.44
 H      -3.029250     5.935792    -3.277801      26.85
 C      -3.074047     2.754612    -3.161383      44.13
 H      -3.007395     2.594707    -4.225750      22.22
 C      -3.546853     1.521975    -0.950161       6.69
 C      -4.086202     0.236898    -0.172746      87.53
 H      -4.686376    -0.208113    -0.819161      26.19
 O      -4.900296     0.821579     0.990105     221.33
 H      -4.395075     0.705883     1.829421      22.76
 C      -3.027487    -0.761489     0.131558      67.43
 H      -2.363930    -0.793988    -0.861063      20.04
 C      -3.569317    -2.122542     0.841940      87.20
 O      -4.648518    -2.923667    -0.007662     123.66
 H      -3.934383    -3.506902    -0.622709      25.43
 H      -4.088036    -1.745577     1.781601      24.16
 H      -2.625431    -2.727410     0.794762      23.45
 C       1.383739    -0.920484    -0.461208      57.68
 H       2.033536    -1.483141    -1.163698      23.69
 C       1.607657     0.687233     1.459857      71.06
 H       2.072791     1.546485     1.957326      19.26
 C       0.274128     0.524138     1.749069       4.03
 O      -0.607006     1.152903     2.657582     260.31
 C      -0.797920     2.571364     2.499271      64.53
 H       0.325254     2.923932     2.843860      18.63
 H      -1.262804     2.832720     1.361021      15.78
 H      -1.499217     2.773072     3.335474      21.08
 C      -0.513352    -0.364189     0.815388      13.96
 O      -1.866496    -0.472862     1.129862     191.43
 C       0.031915    -1.012533    -0.291524      34.67
 H      -0.506844    -1.307535    -1.137784      20.31
 C       2.319065    -0.015559     0.409931      41.64
 C       3.764061     0.244018    -0.103760      77.12
 H       3.894852    -0.161766    -1.173077      24.47
 O       3.830678     1.649925    -0.405484     191.82
 H       4.142597     2.215543     0.418966      23.10
 C       4.901271    -0.287114     0.770418      88.92
 H       4.768373     0.362211     1.731270      23.96
 O       4.756832    -1.685796     1.113270     271.54
 H       5.226278    -2.218983     0.379018      29.19
 C       6.415324    -0.112926    -0.083047      92.93
 O       6.951128     1.271397    -0.092977     180.10
 H       7.252221     1.554510     0.864425      27.25
 H       6.326854    -0.418802    -1.073725      30.65
 H       6.919793    -0.631886     0.682379      29.78
55
name= lig-ACN-Water-frame_639
 C      -3.487481     1.628967    -2.380023      56.74
 H      -3.588527     0.593371    -2.887134      21.35
 C      -3.243931     2.813076    -0.415319      62.60
 H      -3.177237     3.165774     0.757464      16.28
 C      -2.984890     3.990356    -1.102696      -0.87
 O      -2.724303     5.269883    -0.572226     237.83
 C      -2.598859     5.437712     0.878716     100.89
 H      -3.663994     5.245091     1.301275      26.45
 H      -2.269939     6.378370     0.913943      23.44
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 H      -1.812181     4.760873     1.402090      24.82
 C      -2.838847     4.014516    -2.605611       5.10
 O      -2.384674     4.990009    -3.391334      34.26
 H      -2.861210     5.894503    -3.260197      20.48
 C      -3.188318     2.718983    -3.118181      60.98
 H      -3.082263     2.573162    -4.118593      23.66
 C      -3.554968     1.617758    -0.961016      44.55
 C      -4.048946     0.430767    -0.192302      92.16
 H      -4.634550    -0.113511    -0.752655      26.93
 O      -4.872740     0.759933     0.961785     247.96
 H      -4.562994     0.375064     1.800854      23.58
 C      -2.920694    -0.847897     0.078978      72.26
 H      -2.593393    -1.263498    -0.961075      20.28
 C      -3.551784    -2.254767     0.703312     106.88
 O      -4.595787    -3.015330    -0.044423     231.69
 H      -4.088363    -3.535020    -0.701319      30.03
 H      -4.049527    -2.168729     1.721612      24.96
 H      -2.760716    -3.022548     1.149471      23.85
 C       1.605797    -0.815833    -0.385535      46.27
 H       1.880703    -1.235880    -1.415262      19.25
 C       1.591312     0.838375     1.495004      50.97
 H       1.984794     1.693982     1.886776      19.00
 C       0.167134     0.428496     1.712304     -12.76
 O      -0.666129     1.024470     2.729661     229.62
 C      -0.703949     2.520338     2.582961      76.79
 H       0.158261     3.307578     2.927147      21.10
 H      -0.862001     2.823203     1.426577      18.77
 H      -1.667202     3.012506     2.964309      22.01
 C      -0.538898    -0.302498     0.785614      14.70
 O      -1.913007    -0.490155     1.162543     207.46
 C       0.140001    -0.953184    -0.281736      61.04
 H      -0.408238    -1.715750    -0.844608      18.52
 C       2.222640    -0.019091     0.440877      39.45
 C       3.662917     0.204229    -0.110211      66.91
 H       3.694233    -0.428323    -1.086058      24.84
 O       3.848619     1.661990    -0.372393     222.99
 H       4.111596     2.030385     0.509206      25.59
 C       4.909693    -0.342309     0.759696      86.02
 H       5.230901     0.083786     1.740120      25.62
 O       4.731293    -1.787067     1.116750     223.14
 H       4.949310    -2.361167     0.217493      26.83
 C       6.332399    -0.168043    -0.100297      91.13
 O       6.911387     1.348936    -0.086739     109.55
 H       7.006799     1.309020     0.947740      26.38
 H       6.443643    -0.671473    -0.969066      30.98
 H       7.139544    -0.677537     0.367864      30.87
55
name= lig-ACN-Water-frame_640
 C      -3.717402     1.545321    -2.442292      31.28
 H      -3.800868     0.547042    -3.034432      22.09
 C      -3.176789     2.945858    -0.268646      43.04
 H      -3.537900     2.703892     0.859530      16.03
 C      -2.835950     4.038632    -1.125929      16.89
 O      -2.811640     5.275762    -0.613128     209.55
 C      -2.550765     5.497199     0.842355      68.62
 H      -3.498998     5.308043     1.517176      24.61
 H      -2.205009     6.364064     1.067145      23.58
 H      -1.766360     4.633322     1.065689      25.95
 C      -2.924169     3.876913    -2.502273       8.89
 O      -2.322459     5.008670    -3.405096     210.81
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 H      -2.668896     5.836514    -3.139641      26.10
 C      -3.232683     2.732706    -3.217479      41.75
 H      -3.176699     2.783942    -4.217324      21.96
 C      -3.547284     1.716773    -1.019700     -44.08
 C      -3.987053     0.337468    -0.173521      81.52
 H      -4.564655    -0.008307    -0.867706      27.87
 O      -4.839398     0.698589     0.920430     229.99
 H      -4.409925     0.436385     1.778909      23.90
 C      -2.926018    -0.991738     0.131336      77.49
 H      -2.298979    -0.999143    -0.805516      23.64
 C      -3.588331    -2.305404     0.651177     104.47
 O      -4.519465    -3.050962    -0.102691     299.99
 H      -3.978804    -3.586849    -0.591960      32.27
 H      -4.107177    -1.899492     1.537912      24.88
 H      -2.527430    -2.888400     0.723393      23.03
 C       1.501012    -0.783120    -0.398415      35.12
 H       2.228692    -1.274577    -1.127042      20.50
 C       1.473468     0.793714     1.451323      80.17
 H       1.992230     1.277439     2.136867      24.73
 C       0.115809     0.525439     1.712653       5.90
 O      -0.621955     1.004213     2.780467     269.68
 C      -0.683469     2.444908     2.637478      79.11
 H       0.033971     2.658094     3.539832      21.11
 H      -0.296102     2.698139     1.595321      22.38
 H      -1.810520     2.687764     2.904617      21.83
 C      -0.620317    -0.365859     0.787137      13.04
 O      -1.956277    -0.515270     1.048017     212.43
 C       0.188136    -0.984745    -0.221308      27.12
 H      -0.222289    -1.818299    -0.860234      20.51
 C       2.272895     0.145060     0.517766      40.70
 C       3.660058     0.264177     0.027863      75.53
 H       3.646798    -0.156479    -1.074574      21.83
 O       3.903055     1.647873    -0.335010     261.07
 H       4.193411     2.150938     0.429571      26.11
 C       5.002403    -0.448916     0.671641      92.41
 H       4.894970     0.110180     1.589553      24.51
 O       4.743902    -1.833439     1.055163     310.96
 H       4.317563    -2.323876     0.330903      29.48
 C       6.304614    -0.151663    -0.013902     110.91
 O       6.780501     1.248194    -0.061720     148.63
 H       6.978143     1.721889     0.742906      30.98
 H       6.014975    -0.103710    -0.954096      33.51
 H       6.981888    -0.854242     0.390772      31.18
55
name= lig-ACN-Water-frame_641
 C      -3.724409     1.653282    -2.431122      53.16
 H      -4.109132     0.687725    -2.786226      24.47
 C      -3.208211     2.841597    -0.329467      53.72
 H      -3.196907     3.168802     0.794822      14.89
 C      -2.863027     4.021924    -1.041173     -22.22
 O      -2.844737     5.440283    -0.610986     225.27
 C      -2.496559     5.466522     0.763485     119.12
 H      -3.412021     5.386699     1.458506      25.96
 H      -2.073116     6.365253     0.753812      22.07
 H      -1.577075     4.759411     1.187886      21.96
 C      -2.828330     3.932758    -2.599789     -16.61
 O      -2.324998     4.887541    -3.311429      46.19
 H      -2.852625     5.689236    -3.304976      18.66
 C      -3.352439     2.693499    -3.252752      56.35
 H      -3.361228     2.626228    -4.305433      21.15
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 C      -3.555822     1.585039    -0.995800      16.26
 C      -3.937616     0.206373    -0.301770      75.51
 H      -4.543806    -0.341722    -0.844736      28.69
 O      -4.809792     0.629900     0.904356     160.71
 H      -4.433702     0.397795     1.857685      19.77
 C      -2.977801    -0.889846    -0.032117      88.00
 H      -2.639652    -1.275053    -1.026419      24.07
 C      -3.533964    -2.214149     0.701196     101.75
 O      -4.502113    -3.055436    -0.170464     216.90
 H      -3.958082    -3.539994    -0.756837      30.20
 H      -3.957675    -2.160068     1.684079      25.54
 H      -2.680206    -3.011577     1.092932      23.05
 C       1.477955    -0.717798    -0.326457     101.36
 H       1.913991    -1.451754    -1.000253      24.44
 C       1.434401     0.739165     1.568481      46.26
 H       1.786914     1.221740     2.360949      18.63
 C       0.049056     0.485713     1.605454       6.56
 O      -0.552185     0.964212     2.786694     247.62
 C      -0.657088     2.408487     2.843793      95.69
 H      -0.395441     3.033749     3.761188      22.22
 H      -0.167616     2.902142     2.062596      24.27
 H      -1.760993     2.761697     2.513300      18.96
 C      -0.613496    -0.416158     0.791901      18.62
 O      -1.979950    -0.539500     1.037107     204.16
 C       0.071887    -1.116074    -0.165361      42.99
 H      -0.480262    -1.654755    -1.007584      15.85
 C       2.200003     0.142311     0.460576      26.09
 C       3.806343     0.343100     0.024733      62.39
 H       3.745502    -0.242992    -0.999556      21.29
 O       4.007944     1.702295    -0.274155     264.76
 H       4.362225     2.214436     0.523550      21.61
 C       4.864107    -0.396264     0.839193      91.75
 H       5.127798    -0.118048     1.824434      22.25
 O       4.761140    -1.855024     0.959145     319.70
 H       4.360004    -2.232882     0.204918      28.77
 C       6.235011    -0.152373    -0.075358     115.95
 O       6.683125     1.195941    -0.002557     265.33
 H       6.824122     1.252057     0.937280      31.46
 H       6.155000    -0.581563    -0.995124      33.18
 H       7.062713    -0.789406     0.175572      31.57
55
name= lig-ACN-Water-frame_642
 C      -3.692712     1.642496    -2.349229      47.53
 H      -3.916739     0.833047    -3.004920      22.59
 C      -3.225056     2.770138    -0.407369      47.10
 H      -3.104251     2.626898     0.676162      16.86
 C      -3.036285     4.013347    -1.215639      -6.82
 O      -2.842671     5.343144    -0.668720     234.15
 C      -2.399141     5.589509     0.770930      77.73
 H      -3.271661     5.349196     1.421548      24.15
 H      -2.070214     6.560769     1.078345      22.23
 H      -1.607920     4.643637     0.906636      24.86
 C      -2.846363     3.817011    -2.527030      35.83
 O      -2.296618     4.902839    -3.339723     144.84
 H      -2.814067     5.797025    -3.144401      25.81
 C      -3.393699     2.787470    -3.139063      57.49
 H      -3.468359     2.627889    -4.249064      21.46
 C      -3.551955     1.514294    -0.971503      30.36
 C      -4.068185     0.219334    -0.327490     104.08
 H      -4.668817    -0.107021    -1.041409      28.11
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 O      -4.775657     0.520060     0.819516     224.05
 H      -4.344128     0.222863     1.704181      20.65
 C      -2.957479    -0.935140    -0.057426      87.93
 H      -2.412653    -1.201641    -0.963643      23.57
 C      -3.580681    -2.189524     0.677674      98.92
 O      -4.465877    -2.977700    -0.159280     171.26
 H      -3.789512    -3.487873    -0.811278      26.39
 H      -4.196318    -1.813719     1.417966      25.84
 H      -2.482465    -2.696459     0.875000      21.96
 C       1.400075    -0.868446    -0.367838      43.65
 H       1.890208    -1.087807    -1.251375      15.46
 C       1.519906     0.653428     1.588456      20.24
 H       1.952731     1.399498     2.197202      17.10
 C       0.074768     0.438028     1.666294      11.41
 O      -0.533085     0.948349     2.820009     221.55
 C      -0.695822     2.491403     2.985229      93.20
 H      -0.632683     2.552424     4.033391      23.86
 H       0.091527     2.887686     2.522554      26.41
 H      -1.847928     2.762980     2.642902      16.93
 C      -0.703635    -0.430147     0.793084       9.84
 O      -2.037335    -0.524231     1.014859     194.10
 C       0.043769    -1.151125    -0.204785      58.82
 H      -0.409542    -1.961651    -0.855411      20.80
 C       2.205654     0.145678     0.483636      40.30
 C       3.668998     0.336044     0.060446      65.69
 H       3.933251    -0.126688    -0.955689      22.73
 O       4.134783     1.809526    -0.210526     179.83
 H       4.425242     2.146322     0.750146      23.20
 C       4.930995    -0.383817     0.897456      84.90
 H       4.992441    -0.006110     1.856799      28.74
 O       4.710157    -1.850081     0.888252     278.20
 H       4.894939    -2.176447    -0.075369      27.48
 C       6.142289    -0.289174    -0.028536     113.76
 O       6.641838     1.195062     0.042432      84.02
 H       6.967660     1.425378     0.972823      31.90
 H       5.914919    -0.458211    -1.053257      34.62
 H       6.814410    -0.894536     0.521104      33.52
55
name= lig-ACN-Water-frame_643
 C      -3.703970     1.475155    -2.464281      56.21
 H      -4.029412     0.584296    -2.927627      21.73
 C      -3.231665     2.774442    -0.351411      87.55
 H      -3.293975     2.960851     0.664726      22.20
 C      -3.108239     3.970861    -1.057756     -10.62
 O      -2.819506     5.224495    -0.702876     224.10
 C      -2.386534     5.530852     0.723840      90.96
 H      -3.124812     5.339861     1.471898      24.07
 H      -2.067549     6.603345     0.439497      22.09
 H      -1.255704     5.030138     1.043399      21.27
 C      -2.895409     3.996957    -2.560976     -14.34
 O      -2.300999     4.919287    -3.375006      94.59
 H      -2.513699     5.904892    -2.985990      20.53
 C      -3.406527     2.697044    -3.120624      41.05
 H      -3.385675     2.810004    -4.297509      20.12
 C      -3.553319     1.558903    -1.066063      34.74
 C      -4.037661     0.207518    -0.393461      91.90
 H      -4.718701    -0.275314    -0.982918      25.51
 O      -4.851733     0.410340     0.828339     208.45
 H      -4.246085     0.592051     1.571869      24.61
 C      -2.972004    -0.943586    -0.068266      92.13
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 H      -2.431052    -1.084491    -0.941190      22.94
 C      -3.600959    -2.136600     0.586849     126.28
 O      -4.443796    -2.947078    -0.169562     224.89
 H      -3.800922    -3.607188    -0.810097      22.63
 H      -4.128900    -1.788777     1.419570      24.93
 H      -2.981685    -2.908900     1.260498      23.23
 C       1.457720    -0.864704    -0.430349      37.42
 H       1.907838    -1.376656    -1.209142      20.99
 C       1.513165     0.599954     1.510208      71.12
 H       2.136328     1.296521     2.161742      18.53
 C       0.140394     0.405249     1.798980       1.66
 O      -0.582847     0.995072     2.865623     275.38
 C      -0.704386     2.396632     3.127856     123.51
 H      -0.848197     2.536518     4.102409      24.60
 H       0.022060     3.035960     2.952631      28.62
 H      -1.687597     2.938570     2.539302      18.83
 C      -0.640944    -0.398536     0.821806       9.07
 O      -2.115094    -0.439679     1.024200     182.41
 C       0.052538    -1.133921    -0.202875      37.04
 H      -0.399350    -1.986430    -0.725586      16.12
 C       2.166800    -0.019373     0.413453      38.23
 C       3.655545     0.396427     0.084363      67.06
 H       3.493569     0.173011    -1.002560      21.21
 O       4.121623     1.816346    -0.121648     205.22
 H       4.432480     2.283318     0.785881      22.68
 C       4.786466    -0.447114     0.784361     121.35
 H       4.887786    -0.160989     1.774991      26.44
 O       4.637865    -1.823064     0.889255     289.74
 H       4.709202    -2.372730    -0.078870      23.49
 C       6.194924    -0.197948     0.174389     115.77
 O       6.676076     1.111057     0.012670     175.59
 H       6.802279     1.355587     1.020873      29.93
 H       5.918654    -0.442770    -0.904599      30.92
 H       6.897913    -0.971050     0.227020      33.55
55
name= lig-ACN-Water-frame_644
 C      -3.670147     1.508283    -2.530180      35.86
 H      -3.955526     0.617951    -3.078693      19.73
 C      -3.326094     2.770833    -0.324201      58.52
 H      -3.422080     2.744266     0.669594      15.60
 C      -2.994898     3.917762    -1.146109       9.91
 O      -2.789232     5.191414    -0.591322     245.45
 C      -2.335099     5.540427     0.599029     119.39
 H      -3.060513     5.368585     1.369176      27.79
 H      -2.285257     6.737958     0.788305      21.88
 H      -1.266011     4.923124     0.940820      22.71
 C      -3.086398     3.853396    -2.559695       9.11
 O      -2.347458     4.899290    -3.342899     230.48
 H      -2.732553     5.870034    -3.201088      18.76
 C      -3.325475     2.726174    -3.272507      51.42
 H      -3.286773     2.569264    -4.443758      22.13
 C      -3.634704     1.480060    -1.073042     -10.19
 C      -3.996812     0.176108    -0.371122      88.14
 H      -4.591525    -0.344631    -1.084936      26.23
 O      -4.929740     0.362662     0.827299     126.33
 H      -4.523054     0.704954     1.635276      23.44
 C      -2.922382    -0.835434    -0.099467      86.24
 H      -2.495359    -1.240448    -0.925835      23.31
 C      -3.632258    -2.139878     0.690144      82.11
 O      -4.503678    -3.001863    -0.269002     148.49
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 H      -3.857291    -3.605859    -0.790491      27.12
 H      -4.390051    -1.744709     1.352167      23.36
 H      -2.622204    -2.584042     0.980791      22.23
 C       1.443678    -0.910104    -0.480367      57.08
 H       1.928197    -1.656000    -1.093450      22.20
 C       1.483981     0.588318     1.484935      65.60
 H       2.124019     1.232624     2.288162      16.66
 C       0.076645     0.403077     1.802968       1.24
 O      -0.612053     0.960208     2.903021     269.78
 C      -0.695968     2.394159     3.233251      90.05
 H      -0.963949     2.630718     4.140631      21.94
 H       0.225896     2.704050     3.038375      26.85
 H      -1.557381     2.818765     2.413406      16.47
 C      -0.640072    -0.371558     0.906414       8.00
 O      -1.993647    -0.316783     1.026063     196.28
 C       0.072610    -1.070640    -0.120532      62.23
 H      -0.548505    -1.585832    -0.809866      16.95
 C       2.196230    -0.021900     0.391153      36.53
 C       3.662109     0.388870    -0.091133      70.02
 H       4.016997     0.014106    -1.065852      23.15
 O       3.985094     1.805923     0.006207     233.42
 H       4.321363     2.016759     0.959853      21.88
 C       4.678024    -0.405572     0.814495      86.56
 H       4.509608    -0.055121     1.786239      24.26
 O       4.512097    -1.892402     0.890192     297.25
 H       4.153580    -2.234650    -0.032663      23.59
 C       6.199614    -0.239775     0.080469      87.38
 O       6.796417     1.104496     0.042928     215.83
 H       6.957516     1.467469     0.957883      30.46
 H       6.205341    -0.675329    -1.012651      29.41
 H       6.750384    -0.690039     0.837163      29.50
55
name= lig-ACN-Water-frame_645
 C      -3.649037     1.563601    -2.507229      63.70
 H      -3.704032     0.611918    -3.084246      24.01
 C      -3.440665     2.661972    -0.446932      77.18
 H      -3.303186     2.705708     0.548287      19.14
 C      -2.968219     3.835837    -1.136853     -23.42
 O      -2.813323     5.157143    -0.721058     192.02
 C      -2.284972     5.546592     0.769742      78.48
 H      -2.864385     5.059427     1.506650      28.12
 H      -2.000706     6.756516     0.627767      22.13
 H      -1.108147     5.052493     0.771571      22.74
 C      -3.029744     3.840733    -2.647220     -10.96
 O      -2.487952     4.843324    -3.275270     133.55
 H      -2.973430     5.679623    -3.216244      19.68
 C      -3.308833     2.627614    -3.353969      44.42
 H      -3.013274     2.655401    -4.462491      18.84
 C      -3.705514     1.546816    -1.106513      40.91
 C      -4.075695     0.203453    -0.320833      83.20
 H      -4.632516    -0.391441    -1.054677      26.58
 O      -4.966402     0.375866     0.750679     169.90
 H      -4.422548     0.265430     1.607538      21.62
 C      -2.910110    -0.865795     0.071680     103.77
 H      -2.381667    -0.930011    -0.825552      26.58
 C      -3.641791    -2.120118     0.603696     119.28
 O      -4.461286    -3.008898    -0.295763     229.74
 H      -3.840918    -3.473940    -0.735309      32.41
 H      -4.160971    -1.913572     1.584721      25.09
 H      -3.001778    -2.894875     1.060782      25.68
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 C       1.399768    -0.949073    -0.342652       9.06
 H       1.739267    -1.318434    -1.368105      16.36
 C       1.511501     0.614115     1.503096      47.80
 H       2.122161     1.458514     2.206102      16.71
 C       0.137127     0.505186     1.825627      14.14
 O      -0.636293     0.847353     2.980596     223.95
 C      -0.588022     2.404019     3.155439      85.87
 H      -0.972152     2.516403     4.134532      21.95
 H       0.320510     2.893751     3.114314      25.41
 H      -1.343284     3.108433     2.415093      17.99
 C      -0.606174    -0.375050     0.865520      15.14
 O      -1.981506    -0.228350     0.955484     178.33
 C       0.026829    -1.041250    -0.131376      84.12
 H      -0.474341    -1.639412    -0.835544      22.65
 C       2.191829     0.063628     0.261287      35.99
 C       3.631901     0.295928    -0.114093      90.46
 H       3.544191     0.199211    -1.209289      24.83
 O       3.800748     1.770026     0.088469     252.24
 H       4.297267     2.048642     0.879066      23.73
 C       4.710810    -0.406219     0.707235     106.50
 H       4.829181    -0.012828     1.696143      26.97
 O       4.341223    -1.857299     0.923928     306.96
 H       4.414914    -2.332125     0.073106      30.06
 C       6.157872    -0.299867     0.226318      91.28
 O       6.873833     1.121279     0.027508     160.05
 H       7.148553     1.293784     0.938736      28.87
 H       6.414480    -0.941829    -0.766317      30.63
 H       6.768451    -0.989940     0.803892      32.09
55
name= lig-ACN-Water-frame_646
 C      -3.659188     1.386091    -2.602669      23.29
 H      -3.847035     0.333160    -3.006181      20.27
 C      -3.410523     2.777001    -0.419480      43.30
 H      -3.541856     2.799931     0.650571      20.06
 C      -3.095186     3.832676    -1.211943       8.55
 O      -2.796137     5.153710    -0.713401     219.89
 C      -2.200269     5.408186     0.708115      85.57
 H      -2.846669     5.205454     1.599097      23.14
 H      -2.510257     6.661578     0.692098      22.21
 H      -1.033643     5.034212     0.867743      22.48
 C      -2.904578     3.744723    -2.587434      18.87
 O      -2.597401     4.922014    -3.352566     247.88
 H      -2.729270     5.691121    -2.825018      25.30
 C      -3.266221     2.594660    -3.287232      56.81
 H      -3.147575     2.421888    -4.340289      20.65
 C      -3.794678     1.447834    -1.148132      -7.72
 C      -4.112943     0.169322    -0.413430      92.35
 H      -4.723474    -0.470402    -1.099495      26.08
 O      -4.996108     0.453541     0.748271     142.79
 H      -4.610762     0.285254     1.688448      21.37
 C      -2.976051    -0.817758     0.034719      84.16
 H      -2.512849    -1.242459    -0.847874      22.90
 C      -3.559084    -2.247199     0.631971     109.50
 O      -4.380319    -2.926204    -0.314990     204.01
 H      -3.836311    -3.533499    -0.899555      28.61
 H      -4.407180    -1.922390     1.324559      23.33
 H      -2.690129    -2.742673     0.970587      26.25
 C       1.393913    -0.871525    -0.359709      32.19
 H       1.926668    -1.435100    -1.272372      19.05
 C       1.577538     0.734440     1.478535      72.70
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 H       2.396888     1.465710     2.102068      16.67
 C       0.187021     0.427778     1.775835       0.59
 O      -0.539421     0.922045     2.963167     221.43
 C      -0.499049     2.337493     3.118269      62.15
 H      -0.974727     2.769381     4.129075      20.70
 H       0.544222     2.571174     3.041036      23.99
 H      -1.155095     2.703699     2.131822      20.25
 C      -0.620038    -0.283500     0.862998       5.95
 O      -2.059435    -0.158197     0.998775     145.37
 C      -0.021930    -1.113126    -0.201871      63.46
 H      -0.593823    -1.856371    -0.738224      17.58
 C       2.045597     0.050663     0.393490      35.37
 C       3.529631     0.387119    -0.065081      96.50
 H       3.760851     0.101265    -1.108892      24.59
 O       3.657420     1.757048     0.093605     274.88
 H       4.177181     1.957312     0.869658      25.87
 C       4.712344    -0.479207     0.658539      86.30
 H       4.515497     0.027191     1.615048      26.63
 O       4.234779    -1.757053     0.940775     343.05
 H       4.623965    -2.393144     0.379086      31.81
 C       6.293163    -0.351469     0.276980      94.21
 O       6.824084     0.974427     0.072846     210.63
 H       7.021925     1.397102     0.952142      29.61
 H       6.254518    -0.651872    -0.866534      27.94
 H       6.916419    -0.794773     1.107541      28.78
55
name= lig-ACN-Water-frame_647
 C      -3.686152     1.299651    -2.541238      58.78
 H      -4.018036     0.562925    -3.320759      20.97
 C      -3.493931     2.635770    -0.477192      48.02
 H      -3.750178     2.783502     0.636000      19.27
 C      -3.108531     3.936701    -1.173497     -12.12
 O      -2.763935     5.122798    -0.636864     255.79
 C      -2.263298     5.331906     0.564625      92.07
 H      -2.760141     4.567173     1.278376      21.67
 H      -1.984739     6.563715     0.857539      19.62
 H      -1.074686     4.973124     0.569982      25.47
 C      -2.881671     3.748821    -2.654310      -7.64
 O      -2.650090     4.866461    -3.430605     115.73
 H      -2.820049     5.741892    -2.908688      22.09
 C      -3.203752     2.449685    -3.253025      44.59
 H      -3.213929     2.563056    -4.277645      20.39
 C      -3.753130     1.458860    -1.140183      38.88
 C      -4.183632     0.119652    -0.408151      73.99
 H      -4.856537    -0.474239    -1.136816      23.46
 O      -5.045125     0.549996     0.758971     165.14
 H      -4.425028     0.582350     1.495234      26.07
 C      -3.041551    -0.867775    -0.052244      68.55
 H      -2.316905    -0.885660    -0.943292      21.21
 C      -3.488544    -2.174176     0.691527     112.49
 O      -4.290871    -2.901460    -0.399311     212.36
 H      -3.512050    -3.533887    -0.925910      23.02
 H      -4.011429    -2.133417     1.720766      24.28
 H      -2.701175    -2.745580     0.974789      27.36
 C       1.269542    -0.866826    -0.460004      46.55
 H       1.984422    -1.668815    -0.983222      18.73
 C       1.478407     0.759030     1.487816      49.90
 H       2.083355     1.473213     2.322502      16.03
 C       0.160659     0.440034     1.794450       8.13
 O      -0.395291     0.907445     2.897345     257.38
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 C      -0.367680     2.338896     3.001701      77.49
 H      -1.002269     2.581890     4.059017      20.13
 H       0.561934     2.871252     3.129617      23.01
 H      -0.840559     3.024748     2.117670      20.71
 C      -0.723586    -0.272873     0.794501       3.96
 O      -2.077414    -0.131372     1.031316     130.04
 C      -0.046149    -1.085502    -0.146750      64.19
 H      -0.563447    -1.833982    -0.787731      20.02
 C       2.144242     0.007288     0.440922       7.33
 C       3.494446     0.359788    -0.072076      81.81
 H       3.401574     0.224828    -1.158844      20.38
 O       3.631659     1.848010     0.086645     265.05
 H       3.928234     2.066503     1.039006      21.49
 C       4.631447    -0.342900     0.827093      85.77
 H       4.861486     0.036490     1.854684      22.01
 O       4.196721    -1.772528     0.964430     304.71
 H       4.422943    -2.184191     0.012820      23.93
 C       6.268974    -0.435335     0.207726      93.27
 O       6.757108     0.909539     0.144228     234.41
 H       6.838245     1.186493     1.153128      27.97
 H       6.665385    -1.197839    -0.603717      28.85
 H       6.765702    -1.108649     1.027697      29.66
55
name= lig-ACN-Water-frame_648
 C      -3.650117     1.398898    -2.544147      48.88
 H      -3.934515     0.371335    -2.825576      18.78
 C      -3.560425     2.676760    -0.548801      53.46
 H      -3.616729     2.597723     0.638200      12.87
 C      -3.054643     3.733560    -1.219443      18.91
 O      -2.862750     5.148589    -0.786616     215.20
 C      -2.123292     5.156044     0.645845      91.97
 H      -2.706112     4.710384     1.595646      23.68
 H      -2.388366     6.398403     0.941318      24.19
 H      -1.042640     4.770098     0.450507      23.86
 C      -3.013217     3.729890    -2.610835       8.48
 O      -2.663550     4.732275    -3.518903     156.07
 H      -3.068848     5.698762    -3.331757      21.79
 C      -3.160417     2.492135    -3.258621      59.56
 H      -3.015057     2.280587    -4.277524      25.72
 C      -3.739282     1.332344    -1.134953       9.77
 C      -4.287457     0.210283    -0.322777      81.80
 H      -5.039562    -0.456742    -0.972338      22.20
 O      -5.046951     0.604483     0.756955     208.12
 H      -4.578532     0.715531     1.594046      24.40
 C      -3.017034    -0.793579     0.061106      83.89
 H      -2.660339    -1.150624    -1.034617      18.67
 C      -3.394273    -2.148405     0.581299     121.45
 O      -4.177084    -2.895510    -0.412869     232.23
 H      -3.433354    -3.494356    -0.906226      24.96
 H      -4.088808    -1.880963     1.446195      23.71
 H      -2.550308    -2.658687     0.815796      27.16
 C       1.333402    -0.870915    -0.324703      57.77
 H       1.528126    -1.413926    -1.327693      10.70
 C       1.453596     0.578299     1.418140      47.01
 H       1.977815     1.330949     2.167618      15.03
 C       0.056320     0.425542     1.626543      19.32
 O      -0.346353     0.940890     2.919213     220.91
 C      -0.266423     2.473124     2.959340      56.77
 H      -1.125497     2.668716     3.895278      18.09
 H       0.769413     2.780048     3.190916      22.06
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 H      -0.760302     2.772757     1.990131      18.70
 C      -0.751729    -0.257101     0.833119      22.10
 O      -2.130203    -0.165497     0.959455     202.89
 C      -0.113359    -1.026729    -0.146370     108.26
 H      -0.703070    -1.748037    -0.786799      15.12
 C       2.070172     0.000929     0.352178      57.21
 C       3.567312     0.427349     0.050618      83.79
 H       3.894376     0.120107    -0.957988      24.66
 O       3.664967     1.926503     0.058142     208.62
 H       3.995560     2.196603     1.036349      20.70
 C       4.679600    -0.391127     0.788572      90.80
 H       4.630446     0.129161     1.818624      24.34
 O       4.211540    -1.770219     0.975707     267.65
 H       4.064767    -2.174078    -0.025435      25.41
 C       6.047724    -0.545495     0.304121      91.10
 O       6.730827     0.859005     0.201254     213.26
 H       7.204818     1.137167     1.066256      29.40
 H       5.953309    -0.810166    -0.801647      30.44
 H       6.709555    -1.084873     1.133836      27.97
55
name= lig-ACN-Water-frame_649
 C      -3.593210     1.297215    -2.534080      81.84
 H      -3.520581     0.537964    -3.255451      21.73
 C      -3.534089     2.624503    -0.450285      60.31
 H      -3.643643     2.917487     0.671002      12.89
 C      -3.066990     3.797929    -1.306024       6.92
 O      -2.928194     5.022359    -0.773147     261.47
 C      -2.095806     5.073628     0.603349      87.19
 H      -2.694214     4.290869     1.256431      19.95
 H      -1.958142     6.339610     0.830031      19.65
 H      -0.991023     4.798130     0.598160      26.05
 C      -3.080156     3.660914    -2.739021       7.18
 O      -2.685985     4.674334    -3.601935     121.22
 H      -2.772622     5.555698    -3.045474      19.33
 C      -3.221150     2.436214    -3.314424      64.14
 H      -2.835251     2.471593    -4.357598      18.87
 C      -3.804624     1.461917    -1.120037      30.72
 C      -4.224722     0.202922    -0.266915      68.60
 H      -4.894824    -0.505421    -1.004510      21.57
 O      -5.119749     0.669369     0.874847     170.11
 H      -4.439034     0.739933     1.644641      23.06
 C      -3.104223    -0.715403    -0.020817      73.83
 H      -2.407918    -0.632639    -1.031245      19.23
 C      -3.381814    -2.158562     0.533397     127.52
 O      -4.077789    -2.935443    -0.438170     292.07
 H      -3.584312    -3.429020    -1.026157      30.18
 H      -4.114779    -2.239934     1.390997      23.45
 H      -2.500894    -2.560695     0.972610      26.91
 C       1.268821    -0.991393    -0.429523      19.40
 H       1.773301    -1.307572    -1.302277      14.02
 C       1.446942     0.499524     1.421246      38.77
 H       2.110276     1.103099     2.090120      16.96
 C       0.076464     0.511965     1.727881      18.12
 O      -0.364959     1.054728     2.906201     280.70
 C      -0.264908     2.466514     2.939817      78.42
 H      -0.894094     3.189088     3.745127      18.57
 H       0.799528     2.798688     3.095247      22.24
 H      -0.387868     2.963981     2.000284      22.63
 C      -0.827963    -0.316424     0.780966      12.91
 O      -2.156381    -0.153485     0.909356     213.06
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 C      -0.117516    -1.013456    -0.208971      70.36
 H      -0.664661    -1.628193    -0.975100      18.51
 C       2.139548     0.036425     0.277728      20.70
 C       3.630729     0.487614     0.006725      73.77
 H       3.710385     0.308489    -1.076372      20.09
 O       3.751974     1.936151     0.070176     241.33
 H       4.245660     2.219182     0.927173      23.88
 C       4.540153    -0.430259     0.957363     110.23
 H       4.600386    -0.209802     2.117768      25.14
 O       4.213370    -1.784048     0.979022     331.27
 H       4.285861    -2.319634     0.147059      28.71
 C       5.999216    -0.396289     0.339658      97.83
 O       6.720105     0.754526     0.225832     252.78
 H       7.127899     0.923105     1.066012      29.84
 H       5.861124    -0.798479    -0.715530      30.78
 H       6.499927    -1.456002     0.572275      30.89
55
name= lig-ACN-Water-frame_650
 C      -3.540288     1.210164    -2.539679      49.71
 H      -3.706454     0.220699    -2.689326      23.70
 C      -3.461087     2.733871    -0.525096      63.54
 H      -3.755505     2.746486     0.525046      20.47
 C      -3.209022     3.767012    -1.316655       8.00
 O      -2.877465     4.985515    -0.656507     298.96
 C      -2.115120     4.992087     0.423582      94.58
 H      -2.510119     4.485852     1.409867      19.28
 H      -2.187959     6.169932     0.938708      20.66
 H      -1.161448     4.545014     0.068548      24.72
 C      -3.038907     3.657774    -2.780536       6.89
 O      -2.725685     4.714310    -3.634783     237.41
 H      -2.385677     5.470567    -3.196100      27.48
 C      -3.282234     2.315753    -3.375403      40.67
 H      -3.228260     2.032201    -4.511964      18.17
 C      -3.861338     1.466555    -1.140233       6.91
 C      -4.303665     0.303388    -0.275963      68.72
 H      -5.182748    -0.331768    -0.871931      21.18
 O      -5.103957     0.655582     0.964257     172.51
 H      -4.492509     0.852115     1.788103      21.67
 C      -3.066408    -0.746254    -0.076010      55.32
 H      -2.718334    -0.961452    -1.268672      15.84
 C      -3.419737    -2.129821     0.506681     110.83
 O      -4.052624    -3.045670    -0.514668     250.00
 H      -3.295582    -3.357068    -0.993745      27.26
 H      -3.956293    -1.892975     1.415003      23.92
 H      -2.432479    -2.670096     0.663750      21.29
 C       1.355258    -0.894123    -0.595959      42.63
 H       1.621402    -1.714715    -1.076459      18.05
 C       1.491259     0.568214     1.476642      61.40
 H       2.037683     1.053673     2.205088      16.02
 C       0.110108     0.406465     1.712002      -8.74
 O      -0.474692     1.131604     2.889495     207.27
 C      -0.176022     2.590955     2.864743      65.89
 H      -0.984273     2.674865     3.764797      18.00
 H       0.831523     2.850351     3.205451      21.96
 H      -0.552151     2.958902     2.005966      24.33
 C      -0.704459    -0.251091     0.791228      -2.11
 O      -2.140590    -0.078916     0.937838     141.17
 C      -0.119100    -1.048612    -0.300837      73.70
 H      -0.750682    -1.648785    -0.978752      14.97
 C       2.065190    -0.041410     0.246516      31.30
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 C       3.500511     0.414104    -0.033258      70.26
 H       3.933895     0.097472    -0.982762      21.28
 O       3.883751     1.924122     0.103467     185.20
 H       3.988961     2.027562     1.091673      23.77
 C       4.499694    -0.382106     1.039734      85.92
 H       4.351523     0.107430     2.101802      22.05
 O       4.174140    -1.891640     0.991893     293.69
 H       4.566390    -2.106651     0.176485      28.44
 C       5.930376    -0.457436     0.254228      91.25
 O       6.805509     0.765107     0.279263     257.20
 H       7.014359     1.108331     1.178240      32.57
 H       5.662099    -0.536344    -0.794748      29.31
 H       6.622909    -1.119905     0.893621      25.76
55
name= lig-ACN-Water-frame_651
 C      -3.634578     1.194344    -2.453186      66.09
 H      -3.853317     0.387362    -2.996757      28.54
 C      -3.583000     2.683210    -0.595596      63.18
 H      -3.529171     2.831282     0.412992      20.63
 C      -3.196131     3.817267    -1.405221      -5.10
 O      -2.985703     5.034177    -0.778794     258.32
 C      -1.996938     4.910399     0.448244      97.15
 H      -2.412817     4.282357     1.253890      24.63
 H      -1.737875     6.129696     0.572242      21.37
 H      -0.958778     4.611041     0.245019      27.91
 C      -3.036528     3.578216    -2.823178       1.50
 O      -2.753436     4.706163    -3.654251     109.54
 H      -2.913528     5.505869    -3.082637      20.91
 C      -3.297768     2.267029    -3.337996      50.31
 H      -3.206615     2.181510    -4.527869      18.02
 C      -3.815435     1.407733    -1.110958      42.73
 C      -4.395350     0.330575    -0.224277      67.87
 H      -5.227918    -0.300336    -0.943399      21.69
 O      -5.019760     0.621572     0.994651     226.70
 H      -4.301624     0.778620     1.685185      23.20
 C      -3.096194    -0.714237    -0.050187      59.03
 H      -2.346673    -0.820739    -1.071562      19.70
 C      -3.408692    -2.154987     0.421354     115.08
 O      -4.067151    -3.078106    -0.504835     209.30
 H      -3.486660    -3.677418    -1.176454      24.30
 H      -4.132993    -2.267884     1.202088      25.03
 H      -2.425473    -2.512632     0.956732      23.99
 C       1.263052    -0.854002    -0.613573      33.55
 H       1.851781    -1.226818    -1.287206      20.62
 C       1.508387     0.556127     1.414055      67.35
 H       2.102365     1.116102     1.935300      20.35
 C       0.129719     0.409459     1.762105       7.66
 O      -0.517765     1.097766     2.732019     229.57
 C      -0.230913     2.625071     2.876128      62.57
 H      -0.757827     3.083732     3.699305      21.67
 H       0.867835     2.752637     2.914352      24.03
 H      -0.405557     3.100546     2.027134      29.00
 C      -0.681838    -0.251004     0.703470       7.28
 O      -2.045461    -0.070276     0.852705     131.96
 C      -0.061041    -0.986037    -0.299569      72.53
 H      -0.640259    -1.718292    -0.819455      21.55
 C       2.026296     0.036258     0.299571      24.64
 C       3.515176     0.296221     0.064931      84.11
 H       3.568921     0.080752    -1.018120      21.54
 O       3.903133     1.775251     0.089812     210.26
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 H       4.129874     2.052340     0.992871      26.27
 C       4.503289    -0.455356     0.828716     111.40
 H       4.522992    -0.203538     1.959999      25.27
 O       4.170493    -1.868880     1.026781     291.79
 H       4.212994    -2.496503     0.229693      26.99
 C       5.924754    -0.394086     0.365753     105.20
 O       6.837613     0.816066     0.289027     202.54
 H       7.249893     1.060073     1.242191      25.13
 H       5.920536    -0.751020    -0.632961      32.66
 H       6.336905    -1.405624     0.721582      31.62
55
name= lig-ACN-Water-frame_652
 C      -3.766730     1.213596    -2.551963      55.93
 H      -3.898745     0.264789    -2.964466      21.62
 C      -3.654327     2.729432    -0.586908      60.29
 H      -3.809850     2.973697     0.424937      20.97
 C      -3.161892     3.747076    -1.431898       3.82
 O      -3.004081     5.059698    -0.887248     238.82
 C      -1.884799     4.946249     0.370426      79.46
 H      -2.446135     4.455074     1.088159      25.72
 H      -1.750979     5.988964     0.945467      23.08
 H      -1.202898     4.270578    -0.114593      25.19
 C      -3.079504     3.614977    -2.842799      20.05
 O      -2.797134     4.632245    -3.648539     142.36
 H      -3.159618     5.570441    -3.336607      23.30
 C      -3.270336     2.306074    -3.278086      57.70
 H      -3.029326     2.052958    -4.389166      23.90
 C      -3.868316     1.406041    -1.084175     -17.52
 C      -4.254586     0.163605    -0.186630      72.07
 H      -5.119820    -0.557181    -0.812241      22.00
 O      -4.951977     0.620446     1.021338     195.00
 H      -4.428977     0.563508     1.841326      23.28
 C      -3.077719    -0.713280    -0.059942      67.16
 H      -2.848530    -0.647646    -1.322091      18.65
 C      -3.447449    -2.217633     0.447002     106.58
 O      -4.089860    -3.101729    -0.514354     197.70
 H      -3.214850    -3.400256    -1.150335      22.88
 H      -4.074485    -1.911021     1.248575      25.08
 H      -2.468811    -2.862646     0.800962      22.55
 C       1.325720    -0.734873    -0.508223      70.93
 H       1.442916    -1.090687    -1.548067      14.50
 C       1.451648     0.613003     1.490927      50.94
 H       1.970835     1.208750     2.089402      17.80
 C       0.093228     0.484327     1.617790      16.56
 O      -0.592526     1.147672     2.635132     254.20
 C      -0.239361     2.494376     2.820971      97.18
 H      -0.774150     2.666104     3.656073      22.19
 H       0.826894     2.692157     3.196328      21.93
 H      -0.646708     3.081632     2.091310      27.62
 C      -0.690515    -0.263027     0.728991      11.13
 O      -2.072508    -0.078429     0.800271     134.32
 C      -0.098494    -1.013039    -0.319516      64.57
 H      -0.618793    -1.618404    -1.033865      18.61
 C       2.103196     0.048301     0.274092      56.43
 C       3.510820     0.284147    -0.073130     114.35
 H       3.736443    -0.029247    -1.123683      29.63
 O       3.859281     1.600478     0.054525     242.83
 H       4.266183     1.722444     0.922050      25.58
 C       4.552416    -0.568357     0.827162      65.81
 H       4.478863     0.008630     1.813018      26.02
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 O       4.178714    -1.895371     1.029075     270.90
 H       4.114464    -2.211510     0.005218      27.97
 C       6.113870    -0.425444     0.313963     105.88
 O       6.780697     0.801823     0.317105     265.05
 H       7.184569     1.233365     1.223247      24.96
 H       6.118394    -0.719169    -0.700451      34.22
 H       6.710024    -0.942165     1.102070      30.54
55
name= lig-ACN-Water-frame_653
 C      -3.808311     1.271431    -2.499643      60.36
 H      -3.926269     0.236648    -2.888006      20.57
 C      -3.695950     2.709129    -0.559330      51.74
 H      -4.127502     2.873322     0.485573      19.69
 C      -3.208221     3.784059    -1.337601       4.34
 O      -2.893019     5.072086    -0.878621     316.85
 C      -1.992318     4.946504     0.171520     139.10
 H      -2.289154     4.508761     1.044894      29.74
 H      -1.448418     5.970820     0.232370      23.79
 H      -1.065273     4.454460    -0.123732      29.96
 C      -3.126321     3.584344    -2.744137     -11.59
 O      -2.834015     4.626570    -3.735577     164.65
 H      -2.476507     5.454209    -3.177617      20.92
 C      -3.284323     2.273767    -3.374903      59.45
 H      -3.068795     2.152410    -4.441284      24.59
 C      -4.008191     1.421316    -1.154779      14.46
 C      -4.214779     0.159546    -0.168703      63.23
 H      -5.063853    -0.607141    -0.759480      22.79
 O      -4.923253     0.581217     1.027733     205.89
 H      -4.384188     0.514745     1.853138      23.26
 C      -2.980602    -0.871394    -0.098344      78.12
 H      -2.341683    -1.244956    -1.127966      20.71
 C      -3.449002    -2.191923     0.499143     102.67
 O      -4.096043    -3.081163    -0.528923     165.10
 H      -3.389471    -3.434171    -1.227333      25.46
 H      -4.121374    -2.256990     1.347120      25.82
 H      -2.380058    -2.722972     0.874678      23.00
 C       1.248191    -0.738136    -0.547484      43.86
 H       1.981811    -1.215111    -1.348231      20.00
 C       1.506723     0.664289     1.446245      56.00
 H       1.969448     1.202003     2.258431      18.25
 C       0.018052     0.548794     1.484416       2.49
 O      -0.702751     1.110070     2.543935     213.09
 C      -0.306795     2.503552     2.909526      89.46
 H      -0.832717     2.766498     3.716051      24.12
 H       0.847819     2.544020     2.977781      22.25
 H      -0.408230     3.101745     2.022208      24.75
 C      -0.794635    -0.326586     0.689324      13.89
 O      -2.161042    -0.103016     0.798105     170.46
 C      -0.081313    -0.994165    -0.309099      77.36
 H      -0.650738    -1.404373    -1.131818      19.54
 C       2.106028     0.033302     0.354538       8.99
 C       3.623394     0.143528    -0.193373      79.45
 H       3.714068    -0.174779    -1.261010      24.84
 O       3.868081     1.624652     0.004690     149.17
 H       4.008875     1.822602     1.006346      20.56
 C       4.662365    -0.527826     0.838946      90.97
 H       4.515510    -0.179444     1.876742      25.21
 O       4.210674    -1.974276     0.975149     266.14
 H       4.450354    -2.533835     0.129192      27.68
 C       6.226907    -0.565922     0.361019      97.19
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 O       6.710439     0.883528     0.278068     242.52
 H       6.831838     1.203196     1.242176      25.89
 H       6.340481    -1.056451    -0.569831      31.30
 H       6.787021    -1.310422     0.973179      30.83
55
name= lig-ACN-Water-frame_654
 C      -3.775713     1.232688    -2.536614      44.60
 H      -4.004665     0.260700    -3.156195      23.33
 C      -3.804608     2.702699    -0.513110      52.20
 H      -3.701654     2.813729     0.699822      18.65
 C      -3.317146     3.769669    -1.382777     -11.49
 O      -2.901742     5.025138    -0.935956     253.03
 C      -1.838182     5.034710     0.098140     120.68
 H      -2.312793     4.831388     0.976284      27.67
 H      -1.638239     6.128428     0.262605      24.14
 H      -1.093041     4.288740    -0.167223      28.19
 C      -3.092211     3.560702    -2.815053       6.57
 O      -2.846298     4.571151    -3.710522     193.36
 H      -2.470935     5.383796    -3.350368      23.76
 C      -3.386440     2.314335    -3.338365      47.53
 H      -3.254681     2.211901    -4.343452      23.57
 C      -4.044425     1.445330    -1.096580      13.07
 C      -4.317417     0.180785    -0.342338      63.81
 H      -5.271308    -0.428317    -0.954055      20.46
 O      -4.874105     0.472242     1.012816     151.72
 H      -4.155001     0.789960     1.656247      24.24
 C      -3.051772    -0.891991    -0.049506      68.42
 H      -2.510355    -0.958307    -1.172020      23.84
 C      -3.401718    -2.304499     0.521018     112.74
 O      -4.083618    -3.031893    -0.508076     214.39
 H      -3.463944    -3.414421    -1.042758      31.74
 H      -4.157708    -2.014601     1.324696      25.56
 H      -2.442922    -2.903382     1.036480      24.20
 C       1.333151    -0.807592    -0.541816      53.05
 H       1.665224    -1.592529    -1.418267      22.96
 C       1.381639     0.658185     1.326642      54.00
 H       2.126548     1.234116     2.022488      20.77
 C       0.031948     0.570840     1.514967      25.89
 O      -0.798542     1.135705     2.501185     204.74
 C      -0.345342     2.526526     2.923803      87.76
 H      -0.885905     2.815604     3.765753      24.20
 H       0.746137     2.533389     3.370251      24.06
 H      -0.634642     3.318078     2.163439      23.97
 C      -0.776595    -0.255032     0.632275       3.17
 O      -2.155121    -0.201981     0.832356     130.74
 C      -0.135631    -0.968457    -0.415877      66.22
 H      -0.520883    -1.804827    -1.033303      22.20
 C       2.141914    -0.072466     0.310735      17.53
 C       3.688577     0.170784     0.026101     101.97
 H       3.775009    -0.045661    -1.060003      27.03
 O       3.858332     1.665460    -0.090807     136.97
 H       4.150744     2.006112     0.869928      21.51
 C       4.756171    -0.708516     0.748430     122.26
 H       4.742687    -0.211087     1.703741      27.77
 O       4.305910    -2.029448     0.929055     315.24
 H       4.574418    -2.503800     0.152807      32.18
 C       6.200484    -0.579878     0.436201     118.57
 O       6.590125     0.814155     0.223594     242.22
 H       7.194680     1.196715     0.871620      26.93
 H       6.376331    -0.972006    -0.568972      32.34
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 H       6.811540    -1.002620     1.181971      32.73
55
name= lig-ACN-Water-frame_655
 C      -3.812435     1.242029    -2.508217      51.74
 H      -4.025927     0.091432    -2.831547      23.75
 C      -3.810299     2.722317    -0.581746      52.94
 H      -3.703006     3.000997     0.656064      23.62
 C      -3.364368     3.720321    -1.426425      -1.27
 O      -2.962286     5.013482    -1.028362     141.84
 C      -1.735862     5.144971     0.125056      92.70
 H      -2.111917     4.872925     1.079364      26.46
 H      -1.216618     6.048254     0.032329      26.84
 H      -0.969478     4.419242    -0.161987      30.11
 C      -3.173958     3.547053    -2.775990      10.67
 O      -2.803415     4.541734    -3.710703     178.40
 H      -2.947346     5.387193    -3.340195      21.43
 C      -3.479678     2.298206    -3.351827      62.37
 H      -3.376746     2.110918    -4.342356      28.24
 C      -3.955669     1.402634    -1.157942     -24.96
 C      -4.382769     0.106986    -0.298005      80.38
 H      -5.246172    -0.590068    -0.947142      23.76
 O      -4.868959     0.356546     0.954140     147.34
 H      -4.110239     0.823057     1.446238      26.52
 C      -3.150324    -0.811177    -0.119832      70.10
 H      -2.664491    -1.025336    -1.218741      23.29
 C      -3.441009    -2.263649     0.526315     104.68
 O      -4.083297    -3.057093    -0.491777     216.29
 H      -3.391053    -3.311206    -1.120332      29.76
 H      -4.106407    -2.229890     1.488980      24.37
 H      -2.461947    -2.942227     0.871178      23.37
 C       1.324864    -1.037531    -0.578333      41.93
 H       1.896888    -1.561682    -1.499131      21.99
 C       1.406688     0.639985     1.237933      45.28
 H       1.853041     1.580566     1.896772      20.64
 C      -0.066809     0.529331     1.499589      10.28
 O      -0.792173     1.270329     2.493929     197.09
 C      -0.441390     2.517571     2.986583      80.11
 H      -1.139139     2.578304     3.835162      23.13
 H       0.728942     2.672195     3.180480      23.51
 H      -0.569257     3.307089     2.105378      25.00
 C      -0.746286    -0.178284     0.526759       7.92
 O      -2.119018    -0.287193     0.891782     125.89
 C      -0.051985    -0.963855    -0.465240      67.91
 H      -0.776376    -1.663186    -0.953485      23.51
 C       2.130008    -0.125492     0.296626      15.63
 C       3.621628     0.234445     0.041245      96.95
 H       3.815076    -0.188907    -0.965357      27.57
 O       3.798100     1.640770    -0.030035     195.24
 H       4.348789     1.955420     0.716614      25.50
 C       4.733636    -0.705079     0.931529      89.42
 H       4.690451    -0.555371     1.991407      27.75
 O       4.425430    -2.150278     0.884372     303.03
 H       4.309486    -2.368543    -0.041785      30.58
 C       6.241882    -0.584679     0.352039     117.32
 O       6.514171     0.802452     0.173329     226.70
 H       7.031441     1.041455     0.948462      28.03
 H       6.504517    -1.332344    -0.361350      33.64
 H       6.785973    -0.884577     1.211264      32.25
55
name= lig-ACN-Water-frame_656
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 C      -3.873343     1.180439    -2.494332      48.07
 H      -3.982745     0.151815    -3.144224      22.04
 C      -3.740112     2.649407    -0.620892      42.23
 H      -4.242792     2.850853     0.545952      22.38
 C      -3.292290     3.801072    -1.424217     -22.40
 O      -2.929881     5.081402    -0.949998     215.20
 C      -1.761012     5.166652    -0.006036     121.84
 H      -2.033647     5.160141     1.063464      26.47
 H      -1.591216     6.099959    -0.218648      27.61
 H      -1.056529     4.375677    -0.318580      27.55
 C      -3.315522     3.532442    -2.883930     -19.02
 O      -2.771103     4.513637    -3.715521      84.68
 H      -2.592484     5.443982    -3.283510      20.40
 C      -3.553323     2.208171    -3.425913      48.99
 H      -3.392350     2.165759    -4.506581      19.33
 C      -3.966230     1.335045    -1.065350      30.24
 C      -4.256601     0.082254    -0.298534      82.64
 H      -5.161020    -0.558604    -0.925844      21.50
 O      -4.925820     0.336922     1.004702     135.21
 H      -4.326200     0.696211     1.663339      26.86
 C      -3.115688    -0.896655    -0.121110      83.55
 H      -2.531494    -1.043684    -1.104932      25.93
 C      -3.465527    -2.180139     0.446164     109.73
 O      -4.118861    -3.124656    -0.480881     173.66
 H      -3.452883    -3.313087    -1.353828      25.32
 H      -4.181726    -2.239803     1.430514      23.63
 H      -2.351775    -2.428103     0.746353      24.39
 C       1.401707    -1.095993    -0.530495      29.27
 H       1.926466    -1.756723    -1.308432      17.11
 C       1.341382     0.661786     1.236146      64.52
 H       2.150178     1.502353     1.670253      16.44
 C       0.034985     0.646656     1.435201      18.39
 O      -0.749705     1.226918     2.405619     216.01
 C      -0.469478     2.592178     3.010405      77.57
 H      -1.060300     2.789455     4.002003      22.52
 H       0.616084     2.653596     3.421179      23.58
 H      -0.864534     3.495049     2.312063      21.94
 C      -0.811532    -0.213954     0.502388      -2.14
 O      -2.139206    -0.333686     0.827064     148.07
 C      -0.080018    -1.046961    -0.456985     102.97
 H      -0.514153    -1.435614    -1.411413      20.51
 C       2.019395    -0.163527     0.266678      37.35
 C       3.570259     0.066607     0.018198      79.87
 H       3.859843    -0.136106    -1.021195      23.01
 O       3.726869     1.612795     0.108714     173.72
 H       4.063896     1.818748     0.987657      25.94
 C       4.683521    -0.708792     1.022685      83.31
 H       4.614839    -0.425634     2.046230      27.50
 O       4.489104    -2.232528     0.856362     241.67
 H       4.586753    -2.524207    -0.149872      26.37
 C       6.166932    -0.627708     0.473089      99.18
 O       6.534388     0.860496     0.095376     189.65
 H       6.696275     1.424741     0.943091      27.34
 H       6.140581    -0.932572    -0.568814      32.50
 H       6.955365    -1.078500     1.064499      32.35
55
name= lig-ACN-Water-frame_657
 C      -3.895576     1.112751    -2.576840      49.56
 H      -4.136136    -0.016362    -2.879303      22.35
 C      -3.709934     2.654659    -0.598339      37.13
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 H      -3.798883     2.938737     0.658638      16.76
 C      -3.296928     3.724654    -1.469887     -19.68
 O      -2.979744     5.056873    -0.900695     300.11
 C      -1.807179     5.228611    -0.155012     135.44
 H      -2.138927     5.095187     0.931548      26.69
 H      -1.322657     6.032158    -0.263936      29.14
 H      -1.018203     4.466339    -0.333317      29.47
 C      -3.310901     3.594902    -2.860967      -5.47
 O      -2.757117     4.477134    -3.774340     113.35
 H      -2.358968     5.304784    -3.191616      20.98
 C      -3.636729     2.227174    -3.377090      39.76
 H      -3.532771     1.888475    -4.484007      20.80
 C      -3.951207     1.356138    -1.168925     -10.03
 C      -4.229702     0.118693    -0.231566      55.27
 H      -5.056970    -0.550953    -0.895922      24.00
 O      -4.936027     0.378096     1.054929     138.54
 H      -4.262793     0.437437     1.774999      24.35
 C      -3.005988    -0.883398    -0.179629      88.71
 H      -2.674298    -1.002670    -1.235204      25.53
 C      -3.443477    -2.328946     0.416027     109.52
 O      -4.140575    -3.171738    -0.479114     163.25
 H      -3.395045    -3.349249    -1.270934      25.92
 H      -4.221264    -1.806848     1.218759      24.80
 H      -2.765867    -3.046685     0.930196      25.43
 C       1.276124    -1.070161    -0.449546      21.10
 H       1.746017    -1.765884    -1.099761      20.96
 C       1.446256     0.705058     1.174768      56.73
 H       2.002072     1.430040     1.998985      15.61
 C      -0.035858     0.664165     1.285076      10.40
 O      -0.741840     1.250353     2.401893     187.11
 C      -0.460113     2.602598     3.027379      72.70
 H      -1.168866     2.353303     3.961601      19.09
 H       0.702053     2.840652     3.118984      20.35
 H      -0.820315     3.471497     2.242482      19.84
 C      -0.727137    -0.326145     0.499815      13.29
 O      -2.139715    -0.293528     0.750973     183.44
 C      -0.097673    -1.111551    -0.479751      73.20
 H      -0.697898    -1.792628    -1.110210      20.09
 C       2.102278    -0.199840     0.283897      28.61
 C       3.566968     0.002977     0.117237      87.93
 H       3.748483    -0.250328    -0.941848      21.65
 O       3.668791     1.485761     0.243083     182.89
 H       3.896389     1.773288     1.187147      22.42
 C       4.606185    -0.827911     0.923195     107.31
 H       4.341809    -0.605648     1.935755      28.64
 O       4.512763    -2.227323     0.898911     273.74
 H       4.630345    -2.426057    -0.167422      26.35
 C       6.040827    -0.420095     0.484068     108.13
 O       6.553797     0.853069     0.094047     238.66
 H       6.902522     1.369590     0.983932      24.93
 H       5.929766    -0.987968    -0.494037      33.91
 H       6.732301    -1.126862     0.954231      32.37
55
name= lig-ACN-Water-frame_658
 C      -3.933904     1.173783    -2.521162      36.10
 H      -4.157650     0.218289    -3.103278      21.76
 C      -3.651932     2.634284    -0.636025      50.20
 H      -3.320262     2.681017     0.553420      21.17
 C      -3.329058     3.737345    -1.434714      15.38
 O      -3.131366     4.964541    -1.000014     226.31
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 C      -1.756701     5.207729    -0.157061      95.53
 H      -1.878850     5.226931     0.997320      24.79
 H      -1.608263     6.060382    -0.455994      28.30
 H      -1.073976     4.410032    -0.536026      27.24
 C      -3.244540     3.463368    -2.860922      -8.58
 O      -2.747619     4.451623    -3.814334      81.43
 H      -2.819562     5.456141    -3.423633      19.71
 C      -3.689294     2.278235    -3.379713      51.93
 H      -3.596304     2.391255    -4.562703      22.88
 C      -3.942559     1.359638    -1.126008      28.03
 C      -4.278481     0.123873    -0.234834      71.15
 H      -5.189842    -0.515337    -0.794254      24.96
 O      -4.829948     0.437669     1.047582     171.66
 H      -4.182952     0.316165     1.843947      23.77
 C      -2.998150    -0.919566    -0.218815      70.42
 H      -2.497870    -0.929426    -1.149695      30.25
 C      -3.464447    -2.379431     0.464252      93.26
 O      -4.167672    -3.229539    -0.552586     186.84
 H      -3.560082    -3.565321    -1.179290      32.63
 H      -4.353815    -2.413883     1.341687      24.02
 H      -2.570888    -2.682368     0.949853      27.49
 C       1.295149    -1.126236    -0.481983      40.66
 H       1.840732    -1.674341    -1.144004      21.96
 C       1.343834     0.697655     1.171962      76.49
 H       1.874899     1.405592     1.903627      20.01
 C       0.054804     0.647683     1.234161      17.87
 O      -0.732105     1.272355     2.372495     195.14
 C      -0.442978     2.501732     2.933870     105.12
 H      -0.798679     2.758506     4.111532      22.30
 H       0.687863     2.674297     3.223901      23.03
 H      -1.011457     3.436153     2.384485      21.93
 C      -0.774413    -0.330690     0.522192      11.58
 O      -2.049115    -0.222010     0.694503     141.09
 C      -0.164559    -1.174279    -0.392522      84.70
 H      -0.615669    -2.098574    -0.708429      25.91
 C       2.042774    -0.227291     0.389685      28.29
 C       3.520735    -0.011681     0.103217     106.87
 H       3.812076    -0.201911    -0.946978      24.57
 O       3.700782     1.359377     0.324678     203.64
 H       4.219747     1.639992     1.195581      23.31
 C       4.498817    -0.749958     1.001802      94.34
 H       4.480073    -0.536457     2.071268      27.58
 O       4.514310    -2.247169     0.863420     225.55
 H       4.292272    -2.575861    -0.091665      28.14
 C       5.974992    -0.420354     0.345170     102.99
 O       6.573760     0.906052     0.168880     213.44
 H       7.066424     1.183695     1.056204      25.12
 H       6.225575    -0.959501    -0.635192      30.78
 H       6.514433    -0.667049     1.221788      29.64
55
name= lig-ACN-Water-frame_659
 C      -4.029145     1.264852    -2.558601      61.99
 H      -4.327782     0.279897    -2.914202      27.09
 C      -3.536185     2.553865    -0.572553     -14.05
 H      -3.656912     2.815026     0.572464      14.40
 C      -3.341309     3.635972    -1.509376       3.68
 O      -3.143911     4.995342    -0.958033     251.10
 C      -1.854238     5.177117    -0.279575     116.06
 H      -2.068067     5.093323     0.864367      24.97
 H      -1.506333     6.062132    -0.386087      29.67
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 H      -0.978467     4.516664    -0.563294      27.56
 C      -3.185396     3.523026    -2.890741      16.38
 O      -2.801380     4.406158    -3.781362     163.03
 H      -2.664441     5.307425    -3.335431      19.89
 C      -3.677672     2.291139    -3.417488      58.11
 H      -3.843135     1.984004    -4.533465      25.49
 C      -3.949436     1.292189    -1.094537       6.93
 C      -4.230553     0.074807    -0.290626      76.93
 H      -5.161538    -0.459879    -0.874699      25.81
 O      -4.720720     0.482322     1.048226     139.98
 H      -3.958690     0.472295     1.702426      24.17
 C      -3.154440    -0.942859    -0.106453     112.65
 H      -2.841499    -1.235128    -1.013621      32.09
 C      -3.468903    -2.336732     0.395699     124.75
 O      -4.137713    -3.267715    -0.578448     179.42
 H      -3.397364    -3.466273    -1.131164      32.52
 H      -4.054788    -2.166480     1.459671      25.20
 H      -2.617454    -2.909120     0.539808      26.66
 C       1.308149    -1.178586    -0.465340      70.56
 H       1.727550    -1.800564    -1.166788      25.46
 C       1.379054     0.669574     1.239222      59.75
 H       2.024356     1.430552     1.571315      18.66
 C      -0.096925     0.639342     1.370228      23.20
 O      -0.776187     1.208736     2.298815     181.70
 C      -0.353935     2.534680     2.913849      65.17
 H      -0.969444     2.222630     3.951511      19.87
 H       0.798158     2.605613     2.721296      22.13
 H      -0.761963     3.409322     2.194325      22.49
 C      -0.725692    -0.260474     0.493965      -3.15
 O      -2.184110    -0.185044     0.685276     122.99
 C      -0.041492    -1.338978    -0.258013      69.44
 H      -0.671433    -1.894870    -0.942499      25.21
 C       1.943927    -0.285758     0.304054      34.37
 C       3.417795    -0.056886     0.134276     102.33
 H       3.581468    -0.337841    -0.930749      25.01
 O       3.790729     1.384728     0.300067     154.88
 H       4.109789     1.568276     1.325708      20.18
 C       4.574318    -0.743629     0.915665      97.07
 H       4.455550    -0.360767     1.962819      27.68
 O       4.462901    -2.232698     0.833303     273.84
 H       4.255972    -2.258549    -0.066875      32.06
 C       6.032049    -0.489215     0.440945      94.10
 O       6.558740     0.998289     0.175173     213.14
 H       6.860625     1.402334     1.070491      24.96
 H       5.990473    -1.050750    -0.611603      31.13
 H       6.706414    -1.185704     0.923171      32.72
55
name= lig-ACN-Water-frame_660
 C      -4.139918     1.203214    -2.510009      91.95
 H      -4.542900     0.399513    -3.035242      30.27
 C      -3.519680     2.545947    -0.576897      46.64
 H      -3.683466     2.784562     0.465352      20.99
 C      -3.255670     3.619940    -1.434415     -17.12
 O      -3.146109     4.971146    -0.975831     247.06
 C      -1.916394     5.167712    -0.306646     118.24
 H      -2.017007     4.808310     0.810845      24.18
 H      -1.684685     6.121572    -0.393508      26.94
 H      -1.239288     4.396005    -0.773228      27.93
 C      -3.258935     3.446800    -2.897063     -10.57
 O      -2.820540     4.514630    -3.779904     203.65
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 H      -2.249126     5.088550    -3.329412      25.99
 C      -3.690383     2.217216    -3.446774      30.96
 H      -3.602596     2.156269    -4.538885      16.60
 C      -3.882361     1.323098    -1.192128      -9.32
 C      -4.331032     0.071456    -0.237974      56.24
 H      -5.277768    -0.540954    -0.643942      22.51
 O      -4.679841     0.506115     1.038368     220.21
 H      -3.899947     0.736811     1.542286      25.58
 C      -3.160781    -0.951263    -0.189318      89.21
 H      -2.754161    -0.950070    -1.074082      31.92
 C      -3.439181    -2.397024     0.411317     121.11
 O      -4.115631    -3.213731    -0.563804     159.56
 H      -3.479722    -3.350489    -1.459521      27.20
 H      -4.187340    -2.522634     1.329154      25.05
 H      -2.476885    -2.641332     0.789617      26.47
 C       1.297939    -1.320951    -0.421271      53.85
 H       1.847118    -1.960992    -1.128914      19.75
 C       1.322730     0.582985     1.226463      78.10
 H       1.789930     1.280053     1.735817      22.52
 C      -0.032538     0.508487     1.381525       3.16
 O      -0.896256     1.267567     2.310458     190.04
 C      -0.308574     2.452248     2.825128      89.45
 H      -0.538739     2.849298     4.063194      23.75
 H       0.866264     2.484637     3.085871      23.46
 H      -0.791561     3.365090     2.321611      23.13
 C      -0.835414    -0.359901     0.507736       8.40
 O      -2.230267    -0.219713     0.682241     160.36
 C      -0.145771    -1.341615    -0.203075      79.56
 H      -0.669291    -1.974812    -0.942839      25.62
 C       2.028779    -0.203848     0.334679      18.02
 C       3.537861     0.020986     0.084589      93.87
 H       3.690220    -0.096124    -1.015758      25.63
 O       3.789825     1.395049     0.220394     225.46
 H       4.058429     1.760168     1.178791      22.04
 C       4.626800    -0.803501     0.902357      94.56
 H       4.478419    -0.729730     2.029889      27.28
 O       4.381934    -2.170267     0.791506     293.44
 H       4.494202    -2.611691    -0.034428      33.84
 C       6.111414    -0.441055     0.388954      97.69
 O       6.483849     0.902499     0.166082     228.81
 H       6.951414     1.220194     0.966701      27.13
 H       6.098140    -0.675051    -0.762739      31.20
 H       6.867121    -0.964847     1.024418      31.73
55
name= lig-ACN-Water-frame_661
 C      -4.169986     1.130625    -2.650888      46.98
 H      -4.531495     0.177863    -2.931217      28.90
 C      -3.548318     2.551091    -0.630480      65.07
 H      -3.338646     2.553425     0.347654      20.86
 C      -3.235423     3.633424    -1.497857      16.88
 O      -3.203704     4.925974    -1.046746     216.93
 C      -1.865326     5.116895    -0.238894     112.96
 H      -1.873887     4.807351     0.841072      26.93
 H      -1.837089     6.174219    -0.188697      25.79
 H      -0.971672     4.826651    -0.820725      29.60
 C      -3.262734     3.463079    -2.874658      35.18
 O      -2.866843     4.509475    -3.730524     151.85
 H      -2.470171     5.291051    -3.233641      27.27
 C      -3.707145     2.217134    -3.432220      59.25
 H      -3.744222     2.091509    -4.457735      21.94
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 C      -3.963092     1.255972    -1.124833     -70.47
 C      -4.379402     0.134788    -0.246937      66.73
 H      -5.368608    -0.258745    -0.702402      21.19
 O      -4.730620     0.547021     1.093466     194.10
 H      -3.918916     0.721118     1.661235      22.86
 C      -3.117362    -0.936774    -0.256545      86.86
 H      -2.746304    -1.108814    -1.140082      30.96
 C      -3.406648    -2.381807     0.425505     112.42
 O      -4.092546    -3.190990    -0.587198     141.10
 H      -3.404143    -3.137871    -1.480636      26.20
 H      -4.182485    -2.139550     1.247378      25.69
 H      -2.561447    -2.991508     0.744902      26.42
 C       1.263168    -1.255164    -0.237218      42.85
 H       1.688155    -2.096665    -0.921770      26.05
 C       1.286179     0.543409     1.249551      40.88
 H       1.789647     1.125966     1.875354      21.56
 C      -0.162989     0.413513     1.403406      14.56
 O      -0.854411     1.281334     2.262365     200.51
 C      -0.268820     2.490026     2.845116      69.07
 H      -0.965515     2.461811     3.952260      19.90
 H       0.902113     2.274195     2.760748      21.58
 H      -0.290438     3.320461     2.099627      22.85
 C      -0.902958    -0.495054     0.641139      15.16
 O      -2.220153    -0.291307     0.674992     176.65
 C      -0.181371    -1.328385    -0.304956      83.58
 H      -0.687243    -2.270513    -0.622401      21.98
 C       2.105410    -0.359318     0.285392      11.56
 C       3.659269     0.060971     0.019806      81.52
 H       3.981917    -0.248223    -1.001373      27.74
 O       3.716142     1.507229     0.221929     179.16
 H       4.286166     1.672847     1.017669      21.80
 C       4.646107    -0.781343     0.871181      90.08
 H       4.684216    -0.346956     1.937361      26.55
 O       4.314019    -2.247779     0.746457     190.93
 H       4.581125    -2.317317    -0.288575      28.99
 C       6.089364    -0.512678     0.256774      99.74
 O       6.465523     0.897267     0.162499     244.82
 H       6.710879     1.290022     1.004418      27.65
 H       6.311753    -1.292925    -0.526135      31.79
 H       6.766309    -0.932324     1.075918      30.15
55
name= lig-ACN-Water-frame_662
 C      -4.093670     1.143039    -2.573654      52.33
 H      -4.373523     0.283478    -3.201342      21.90
 C      -3.547673     2.453120    -0.681245      49.73
 H      -3.449225     2.690926     0.240479      23.47
 C      -3.337046     3.546937    -1.527722     -16.31
 O      -3.066630     4.935475    -1.002559     240.52
 C      -1.905618     5.198659    -0.223680     109.90
 H      -2.029003     4.473023     0.599872      27.10
 H      -1.864137     6.184058     0.181892      23.44
 H      -1.006113     4.832026    -0.735488      27.77
 C      -3.264639     3.435970    -2.944724       8.60
 O      -2.932677     4.454258    -3.718162     142.12
 H      -2.593560     5.265702    -3.083016      18.41
 C      -3.757685     2.200608    -3.457049      61.29
 H      -3.841463     2.166692    -4.492760      27.04
 C      -4.094306     1.318734    -1.252551      56.14
 C      -4.325644     0.117286    -0.224928      86.42
 H      -5.177887    -0.518891    -0.630087      28.35
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 O      -4.822747     0.561166     1.129539     192.37
 H      -4.112316     0.401341     1.878129      22.57
 C      -3.149143    -0.969336    -0.201984     105.76
 H      -2.779407    -0.962604    -1.115308      32.84
 C      -3.473487    -2.289838     0.348935     127.00
 O      -4.101858    -3.172664    -0.627791     209.36
 H      -3.396152    -3.295985    -1.346035      29.39
 H      -4.081253    -2.208657     1.284042      27.65
 H      -2.483863    -2.697643     0.783915      26.79
 C       1.242209    -1.344101    -0.323039      50.38
 H       1.783508    -2.196853    -0.950841      20.40
 C       1.319273     0.428295     1.242289      75.66
 H       1.788307     1.291743     1.659342      21.45
 C      -0.067760     0.407131     1.425312       2.56
 O      -0.820675     1.256479     2.203244     207.17
 C      -0.186390     2.447537     2.781963     110.52
 H      -0.883024     2.843052     3.865183      22.64
 H       0.760194     2.434325     3.517596      23.77
 H      -0.404937     3.300141     2.215050      25.75
 C      -0.846314    -0.568865     0.660259       2.88
 O      -2.258759    -0.337967     0.679872     165.00
 C      -0.159565    -1.361340    -0.209972      66.91
 H      -0.596115    -2.106666    -0.920566      24.72
 C       2.033251    -0.295850     0.414420      27.63
 C       3.541012     0.006358     0.016847      81.23
 H       3.590530     0.027868    -1.089596      24.56
 O       3.620064     1.580547     0.233742     188.72
 H       4.015268     1.887250     1.059554      25.47
 C       4.677806    -0.745997     0.748716      96.92
 H       4.526172    -0.658936     1.920166      24.76
 O       4.315616    -2.218357     0.698863     247.16
 H       3.937470    -2.557879    -0.250493      25.15
 C       6.098202    -0.693999     0.353341      99.93
 O       6.430735     0.887942     0.081043     133.09
 H       6.831042     1.192901     0.920297      27.78
 H       6.165147    -0.816481    -0.721975      31.79
 H       6.836426    -1.201371     1.109421      31.07
55
name= lig-ACN-Water-frame_663
 C      -4.078014     1.123171    -2.693497     -36.90
 H      -4.470912     0.071616    -2.998354      19.25
 C      -3.612278     2.519196    -0.646768      26.05
 H      -3.768117     2.491421     0.319022      22.01
 C      -3.299286     3.640314    -1.477601      23.66
 O      -3.000492     4.885426    -1.083273     239.36
 C      -1.887435     5.120006    -0.112747     107.49
 H      -1.754954     4.480735     0.698466      29.48
 H      -2.287372     6.104754     0.264155      23.21
 H      -1.018206     5.347529    -0.718126      27.18
 C      -3.366909     3.369076    -2.915021      -3.32
 O      -2.969242     4.465150    -3.778130     164.19
 H      -2.497942     5.147499    -3.202793      20.81
 C      -3.775336     2.208979    -3.535686      75.24
 H      -3.709817     2.006156    -4.621632      25.75
 C      -4.126060     1.233587    -1.138796     -36.39
 C      -4.394159     0.056956    -0.193473     106.43
 H      -5.200726    -0.572137    -0.667777      29.09
 O      -4.901657     0.511939     1.063181     186.82
 H      -4.255647     0.409892     1.854747      22.78
 C      -3.195645    -0.820843    -0.193573      83.76
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 H      -2.856470    -0.992329    -1.133148      31.55
 C      -3.545015    -2.326528     0.331829     118.63
 O      -4.148238    -3.155077    -0.650502     236.11
 H      -3.536195    -3.337733    -1.280108      34.55
 H      -4.270388    -2.406187     1.126039      27.17
 H      -2.495315    -2.768252     0.618995      25.05
 C       1.337249    -1.367089    -0.398629      54.52
 H       1.865650    -1.904400    -1.292117      22.43
 C       1.332880     0.511674     1.367661      46.91
 H       1.838222     1.512880     1.709340      18.36
 C      -0.030900     0.351451     1.433882      21.83
 O      -0.759798     1.274583     2.213238     176.54
 C      -0.204400     2.461131     2.821773      94.49
 H      -1.281940     2.762041     3.487691      20.33
 H       0.877739     2.079928     3.239128      22.85
 H       0.150554     3.075315     2.053787      26.88
 C      -0.821207    -0.511862     0.646506      10.00
 O      -2.150317    -0.328747     0.787898     144.02
 C      -0.101878    -1.501353    -0.174643      75.47
 H      -0.783210    -1.863164    -0.944469      23.33
 C       2.002748    -0.448442     0.347764      13.42
 C       3.339144     0.164537     0.032790     101.14
 H       3.510713    -0.090021    -1.042341      23.99
 O       3.502103     1.556770     0.203857     253.68
 H       3.835708     1.672707     1.099343      25.16
 C       4.530970    -0.860162     0.732225      82.83
 H       4.489318    -0.402354     1.853235      25.28
 O       4.307964    -2.204502     0.646462     295.05
 H       4.060635    -2.302018    -0.281319      31.32
 C       6.099623    -0.564833     0.251711      97.23
 O       6.431042     0.755182     0.094150     254.33
 H       6.849918     1.186865     0.937502      24.17
 H       6.181725    -1.297090    -0.583966      32.62
 H       6.839865    -1.191007     0.962998      30.32
55
name= lig-ACN-Water-frame_664
 C      -4.162881     1.053560    -2.614065      76.58
 H      -4.416212     0.049230    -3.174170      23.38
 C      -3.802670     2.521383    -0.575294      78.24
 H      -3.613903     2.884409     0.371031      20.16
 C      -3.284101     3.519520    -1.514273     -20.33
 O      -2.920810     4.863863    -1.132880     236.55
 C      -1.899088     5.135789    -0.024833      82.77
 H      -1.723003     4.273064     0.509118      29.49
 H      -2.296328     5.891981     0.702161      22.13
 H      -0.956260     5.439992    -0.456790      26.18
 C      -3.396876     3.495249    -2.921340       2.01
 O      -3.019211     4.431100    -3.797210     188.09
 H      -2.675579     5.214549    -3.436975      24.95
 C      -3.776147     2.131261    -3.471874      25.83
 H      -3.722244     2.099752    -4.650180      18.48
 C      -4.042691     1.304162    -1.231474      23.61
 C      -4.475591     0.111852    -0.276857      63.33
 H      -5.226203    -0.505806    -0.769422      25.75
 O      -5.022952     0.438361     1.024841     136.03
 H      -4.310442     0.447701     1.671356      25.45
 C      -3.141697    -0.906200    -0.069065      80.49
 H      -2.679526    -0.732087    -0.999104      27.60
 C      -3.555226    -2.318955     0.359189     120.41
 O      -4.246753    -3.143340    -0.715211     201.40
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 H      -3.585790    -3.170968    -1.472143      29.30
 H      -4.135519    -2.147832     1.191908      27.21
 H      -2.733940    -3.050389     0.831519      24.49
 C       1.278932    -1.340833    -0.406446      76.09
 H       1.664199    -1.724837    -1.372727      15.83
 C       1.360190     0.406040     1.313595      50.69
 H       2.109625     1.145627     1.969108      16.30
 C      -0.022367     0.425064     1.514466      16.82
 O      -0.814071     1.249513     2.231718     217.84
 C      -0.152360     2.386551     2.780965     112.89
 H      -0.904049     3.201405     3.452885      22.67
 H       0.382662     2.208363     3.831182      24.00
 H       0.200931     3.067610     2.059019      26.60
 C      -0.676878    -0.555622     0.617012       3.19
 O      -2.142999    -0.311785     0.848847     133.37
 C      -0.100564    -1.511475    -0.222328      74.31
 H      -0.541107    -2.350043    -0.715680      22.83
 C       1.968122    -0.321655     0.395486      39.26
 C       3.379475     0.051909    -0.064404      79.43
 H       3.506056    -0.008252    -1.182042      23.69
 O       3.412537     1.514604     0.197238     246.32
 H       4.019445     1.885218     0.914931      24.90
 C       4.469503    -0.699968     0.744864      77.48
 H       4.442066    -0.674868     1.958059      24.57
 O       4.247212    -2.243535     0.571698     200.51
 H       4.430965    -2.497690    -0.289657      35.61
 C       5.911010    -0.625013     0.197680     102.64
 O       6.493135     0.749223     0.086948     189.64
 H       6.740158     1.022273     1.080927      26.14
 H       6.176362    -0.959695    -0.811882      32.23
 H       6.423336    -1.033486     1.159617      29.65
55
name= lig-ACN-Water-frame_665
 C      -4.150553     1.138158    -2.559368      47.85
 H      -4.441072     0.102421    -2.955489      19.23
 C      -3.818248     2.618025    -0.685588      64.86
 H      -3.910799     2.488860     0.419314      14.89
 C      -3.312655     3.588706    -1.504759      21.33
 O      -2.804808     4.851469    -1.112851     277.19
 C      -1.967456     5.062939     0.022950      83.18
 H      -1.683710     4.153418     0.389941      32.47
 H      -2.445290     5.607786     0.818110      23.10
 H      -1.118536     5.619781    -0.351330      24.89
 C      -3.413767     3.328824    -2.935002       8.76
 O      -3.084459     4.447816    -3.817787     148.56
 H      -2.927633     5.131875    -3.120919      24.35
 C      -3.784680     2.172268    -3.374569      64.33
 H      -3.882019     1.943221    -4.513402      24.99
 C      -4.133326     1.261188    -1.137228     -13.35
 C      -4.370585     0.073505    -0.321717      90.01
 H      -5.037341    -0.480621    -0.855854      24.69
 O      -5.157406     0.385366     0.976011     128.52
 H      -4.536780     0.675822     1.669419      25.81
 C      -3.067163    -0.929974    -0.074197      71.80
 H      -2.592190    -1.309101    -0.996160      22.46
 C      -3.613683    -2.352807     0.396159      94.80
 O      -4.306941    -3.047706    -0.729034     146.39
 H      -3.510932    -3.116646    -1.526387      24.73
 H      -4.376410    -2.349737     1.039110      25.43
 H      -2.562947    -2.846253     0.736849      23.48
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 C       1.235495    -1.259500    -0.451861     -42.50
 H       1.850430    -1.950842    -0.939615      10.96
 C       1.379366     0.387697     1.403348      70.61
 H       2.031147     1.039847     2.264874      14.65
 C      -0.013143     0.361177     1.433710       2.66
 O      -0.880211     1.234617     2.289723     189.40
 C      -0.139425     2.415897     2.847267      71.09
 H      -1.191673     3.062380     2.866809      18.22
 H       0.543374     2.079592     3.799303      22.20
 H       0.713056     2.635054     2.155196      22.71
 C      -0.830341    -0.552905     0.709497       9.54
 O      -2.150726    -0.361724     0.881034     185.87
 C      -0.138281    -1.450723    -0.205219      67.08
 H      -0.654912    -2.308117    -0.543474      18.13
 C       2.005130    -0.325452     0.241392      67.77
 C       3.401995     0.009277    -0.086915      90.58
 H       3.583694    -0.301031    -1.168681      23.90
 O       3.447057     1.463015     0.152548     172.54
 H       4.087395     1.602279     0.985535      20.47
 C       4.415866    -0.778589     0.653132     117.80
 H       4.195097    -0.365834     1.777874      24.94
 O       4.192038    -2.202581     0.572112     319.26
 H       3.950036    -2.299647    -0.369448      31.45
 C       5.847518    -0.623090     0.280776     104.73
 O       6.499777     0.769982     0.088867     167.24
 H       6.841620     1.204762     0.983918      24.48
 H       5.628668    -0.980014    -0.756289      32.87
 H       6.480179    -1.500810     0.533632      33.17
55
name= lig-ACN-Water-frame_666
 C      -4.152821     1.084292    -2.473840      48.12
 H      -4.486906     0.140870    -2.902022      25.61
 C      -3.786535     2.565593    -0.622311      51.43
 H      -3.832843     3.116168     0.428054      17.65
 C      -3.352645     3.678470    -1.503735      -5.64
 O      -2.763191     4.851028    -1.163447     326.66
 C      -2.001151     4.938159     0.110930     103.74
 H      -1.472369     4.090621     0.441478      28.16
 H      -2.713979     5.249243     0.746570      21.50
 H      -1.316627     5.756822    -0.081665      23.52
 C      -3.330247     3.456577    -2.889640      -1.95
 O      -3.176680     4.432940    -3.730560     198.33
 H      -2.713776     5.341880    -3.410099      22.20
 C      -3.857144     2.097122    -3.458025      34.76
 H      -3.793457     1.933350    -4.551539      21.25
 C      -4.192672     1.339488    -1.113818      61.75
 C      -4.304834    -0.031960    -0.240413      89.34
 H      -4.850284    -0.651370    -0.768170      28.38
 O      -5.198600     0.324199     0.862805     140.39
 H      -4.643854     0.655434     1.664360      23.59
 C      -3.160427    -0.969448    -0.073801      81.98
 H      -2.607358    -0.831089    -1.108595      24.47
 C      -3.685541    -2.358020     0.395890     126.52
 O      -4.271467    -2.945082    -0.725945     171.68
 H      -3.466364    -3.234716    -1.460708      23.25
 H      -4.234569    -2.241860     1.258741      28.27
 H      -2.896403    -3.153929     0.765935      25.47
 C       1.179848    -1.263893    -0.484946      63.20
 H       1.453965    -1.988839    -1.166676      19.09
 C       1.337146     0.329296     1.363423      57.90
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 H       1.996209     1.143757     2.006194      17.31
 C      -0.098302     0.366119     1.506025      11.43
 O      -0.779716     1.167648     2.311726     217.96
 C      -0.155247     2.345697     2.844851     104.62
 H      -0.700497     3.410867     3.017244      22.80
 H      -0.054257     2.209479     4.033936      23.87
 H       0.698696     2.774299     2.146683      21.35
 C      -0.866223    -0.536955     0.728653      13.88
 O      -2.249257    -0.449613     0.898360     191.87
 C      -0.222015    -1.406571    -0.146095      55.77
 H      -0.800175    -2.028870    -0.807576      20.14
 C       1.922671    -0.290202     0.277836      24.78
 C       3.367115     0.051320    -0.171280      77.51
 H       3.532391     0.001297    -1.302216      22.70
 O       3.648939     1.393895     0.069111     236.99
 H       3.957203     1.664063     1.026073      20.65
 C       4.381124    -0.831653     0.798929      59.73
 H       4.266753    -0.642689     1.998380      22.82
 O       4.092720    -2.179265     0.634189     301.73
 H       3.924012    -2.532928    -0.339097      24.24
 C       5.922797    -0.557904     0.098776      99.29
 O       6.436348     0.698440     0.149899     254.54
 H       6.651444     0.980767     1.083837      27.93
 H       5.951896    -0.789341    -0.991369      29.26
 H       6.629008    -1.132200     0.742974      28.15
55
name= lig-ACN-Water-frame_667
 C      -4.180838     1.090263    -2.535967      56.44
 H      -4.392162     0.143934    -2.890215      25.43
 C      -3.730533     2.669217    -0.511452      58.75
 H      -3.647687     2.680550     0.708283      19.31
 C      -3.357725     3.550689    -1.486084      -4.85
 O      -2.706728     4.864339    -1.156675     231.77
 C      -2.100953     4.892430     0.189094     119.05
 H      -1.526950     3.979115     0.147704      31.41
 H      -2.611931     4.758455     0.972687      32.42
 H      -1.476391     5.769221     0.336395      26.88
 C      -3.455104     3.330722    -2.903767      18.77
 O      -3.206526     4.538234    -3.776430     161.85
 H      -2.578653     5.058297    -3.117194      21.60
 C      -3.809152     2.180120    -3.364741      68.02
 H      -3.743283     2.022278    -4.372651      25.64
 C      -4.106883     1.292746    -1.070695     -68.59
 C      -4.466984     0.046214    -0.305599      85.78
 H      -5.043339    -0.427886    -0.918397      26.32
 O      -5.193343     0.245825     0.858598     155.99
 H      -4.614860     0.418747     1.671878      22.57
 C      -3.191736    -0.944814    -0.014265      71.63
 H      -2.717960    -1.126811    -1.118466      25.62
 C      -3.631002    -2.318514     0.406163     116.25
 O      -4.321875    -2.944664    -0.768077     184.03
 H      -3.540270    -3.111738    -1.419433      27.13
 H      -4.464008    -2.232730     1.064425      25.25
 H      -2.674706    -2.787872     0.786874      24.69
 C       1.046590    -1.282748    -0.477214      45.47
 H       1.504386    -1.406799    -1.398955      18.46
 C       1.248967     0.368731     1.268935      66.77
 H       1.884340     1.195381     1.744316      19.05
 C      -0.084427     0.313256     1.571587      19.18
 O      -0.763505     1.181931     2.411987     203.49
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 C      -0.147109     2.364956     2.902731      91.72
 H      -1.098014     3.003829     2.561822      20.09
 H       0.120030     2.227670     4.107604      23.27
 H       0.985128     2.569311     2.558494      21.55
 C      -0.924782    -0.543978     0.732907       5.66
 O      -2.295029    -0.488915     0.995940     159.65
 C      -0.301387    -1.391743    -0.197434      77.76
 H      -0.897846    -2.018384    -0.896129      23.29
 C       1.857333    -0.339753     0.239449      24.84
 C       3.370467     0.004063    -0.038298      77.74
 H       3.501298    -0.434846    -1.086086      22.94
 O       3.857086     1.488920    -0.050091     195.48
 H       4.226168     1.674189     0.868041      20.89
 C       4.451501    -0.786233     0.637071      86.02
 H       4.562706    -0.412225     1.761304      24.77
 O       3.979632    -2.281696     0.731954     243.68
 H       4.508118    -2.533047    -0.125265      28.20
 C       5.893460    -0.655799     0.072605     105.93
 O       6.399335     0.789729     0.182065     237.44
 H       6.744582     0.946237     1.108971      28.62
 H       5.995153    -1.084836    -0.948062      32.34
 H       6.449898    -1.406284     0.668072      31.84
55
name= lig-ACN-Water-frame_668
 C      -4.148801     1.168802    -2.460665      84.30
 H      -4.424878     0.269418    -2.847280      24.68
 C      -3.695143     2.478617    -0.529844      75.79
 H      -3.485478     2.579602     0.648602      19.67
 C      -3.243671     3.638258    -1.420681     -10.56
 O      -2.736930     4.805074    -1.100732     234.70
 C      -2.157970     4.759981     0.239253     138.33
 H      -1.204998     4.215990     0.281623      26.15
 H      -2.859940     4.597877     0.820658      30.44
 H      -1.890168     5.837744     0.342553      25.00
 C      -3.526061     3.542107    -2.861530      -9.85
 O      -3.201302     4.519522    -3.714540     203.64
 H      -2.779084     5.284252    -3.328352      24.15
 C      -3.805571     2.107297    -3.419844      44.79
 H      -3.856620     1.954284    -4.420768      23.83
 C      -4.027100     1.341749    -1.106551      55.50
 C      -4.483448     0.074965    -0.371601      79.45
 H      -5.131919    -0.438604    -0.921296      25.82
 O      -5.239892     0.211362     0.975160     100.89
 H      -4.637526     0.300462     1.728990      23.03
 C      -3.289771    -0.882116    -0.068415      49.16
 H      -2.437088    -0.956379    -0.952066      21.00
 C      -3.689287    -2.312560     0.361701     124.01
 O      -4.321827    -2.982692    -0.772883     254.97
 H      -3.769857    -3.109745    -1.457766      34.29
 H      -4.329290    -2.403923     1.305154      24.28
 H      -2.887610    -2.968800     0.653458      26.73
 C       1.060902    -1.198858    -0.573216      62.66
 H       1.336068    -1.942491    -1.339137      23.36
 C       1.227486     0.510796     1.252810      76.97
 H       1.845696     1.162086     1.802939      21.07
 C      -0.147676     0.275334     1.552086       8.34
 O      -0.783264     1.115587     2.523122     186.03
 C      -0.145639     2.406579     2.994065      82.25
 H      -0.703976     3.476168     2.853098      23.38
 H      -0.223687     2.429403     4.240533      23.10
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 H       0.841348     2.638345     2.365753      21.79
 C      -0.979544    -0.582327     0.818355       9.43
 O      -2.319363    -0.449994     1.107001     120.04
 C      -0.411519    -1.364183    -0.302684      55.24
 H      -1.062804    -2.133569    -0.848743      17.79
 C       1.913511    -0.338937     0.255845      43.18
 C       3.387225    -0.027717    -0.098963      79.37
 H       3.399768    -0.088823    -1.241037      23.73
 O       3.905599     1.476483    -0.189808     185.02
 H       4.380776     1.711580     0.607224      24.12
 C       4.471323    -0.872057     0.629699      93.07
 H       4.534966    -0.464719     1.727333      24.20
 O       4.000117    -2.254416     0.794614     289.42
 H       4.165130    -2.923359     0.122414      30.90
 C       5.887644    -0.721336     0.105247     105.96
 O       6.377800     0.749499     0.151337     184.98
 H       6.878984     1.002866     0.982767      29.00
 H       5.936088    -0.769122    -0.991599      31.42
 H       6.612703    -1.299317     0.655750      31.60
55
name= lig-ACN-Water-frame_669
 C      -4.112513     1.156588    -2.543714      42.92
 H      -4.502262     0.258331    -2.979001      25.83
 C      -3.488954     2.531335    -0.593856      60.97
 H      -3.425119     2.677492     0.518854      22.39
 C      -3.308599     3.526551    -1.457682      22.04
 O      -2.730740     4.782002    -0.975710     270.57
 C      -2.202290     4.796293     0.323991     113.03
 H      -1.289881     4.140724     0.457517      26.13
 H      -2.701727     4.322339     0.978101      29.14
 H      -2.058354     5.827114     0.722535      22.45
 C      -3.509733     3.474598    -2.800775      32.25
 O      -3.186344     4.541485    -3.704407     188.15
 H      -2.920381     5.363271    -3.236213      23.07
 C      -3.818017     2.335096    -3.379173      45.69
 H      -3.744385     2.150396    -4.446255      15.89
 C      -4.111400     1.269233    -1.093886     -22.83
 C      -4.452538     0.043793    -0.176535     113.80
 H      -5.017310    -0.506073    -0.856592      25.79
 O      -5.275769     0.230646     0.980326     220.03
 H      -4.729935     0.374992     1.779746      24.62
 C      -3.273790    -0.891449    -0.009270      57.47
 H      -2.810675    -0.666542    -1.138979      20.47
 C      -3.718850    -2.368855     0.280770     112.46
 O      -4.385816    -3.034484    -0.787231     257.21
 H      -3.656281    -3.181338    -1.350115      30.93
 H      -4.472144    -2.188663     1.167716      23.80
 H      -2.803935    -2.773161     0.514544      27.14
 C       0.996566    -1.133448    -0.554761      38.05
 H       1.628769    -1.909530    -1.090100      18.70
 C       1.256331     0.500105     1.219488      69.12
 H       1.750015     1.144746     1.795158      20.14
 C      -0.148764     0.415921     1.570865       1.91
 O      -0.805374     1.099491     2.636651     195.18
 C      -0.194182     2.400451     3.037281      92.08
 H      -1.006580     3.155777     2.638620      20.93
 H       0.027363     2.265908     4.314353      21.63
 H       0.946429     2.487276     2.808397      22.84
 C      -0.980417    -0.583597     0.812433       7.13
 O      -2.438296    -0.420965     1.111638     148.00
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 C      -0.336955    -1.240878    -0.271014      76.65
 H      -0.826305    -2.065456    -0.888998      21.13
 C       1.840262    -0.249999     0.201932      28.84
 C       3.438189     0.013618    -0.331460      61.58
 H       3.512539    -0.505538    -1.363961      22.62
 O       3.810709     1.360117    -0.281200     217.46
 H       4.088664     1.557522     0.651279      23.29
 C       4.424633    -0.912678     0.743365      82.34
 H       4.303445    -0.498234     1.807213      24.47
 O       4.052658    -2.265289     0.854912     320.11
 H       3.926887    -2.367588    -0.086538      29.61
 C       5.968378    -0.665893     0.061333     109.39
 O       6.401271     0.634774     0.121394     229.21
 H       6.559533     0.776564     1.123361      27.75
 H       5.897392    -1.143574    -0.923725      32.31
 H       6.635601    -1.349361     0.572913      31.72
55
name= lig-ACN-Water-frame_670
 C      -4.163904     1.183584    -2.557829      62.38
 H      -4.403060     0.272195    -3.184458      24.40
 C      -3.459968     2.380135    -0.590288      61.82
 H      -3.263934     2.462236     0.427110      21.36
 C      -3.242047     3.628041    -1.375163       7.11
 O      -2.757255     4.776612    -0.899907     262.98
 C      -2.220285     4.792871     0.545272     126.25
 H      -1.177250     4.518105     0.250395      22.14
 H      -2.779352     4.435547     1.233410      27.46
 H      -2.069344     5.907361     0.702589      23.34
 C      -3.383462     3.570227    -2.854650      -4.31
 O      -3.187232     4.588704    -3.681262     177.01
 H      -2.723699     5.387842    -3.108117      21.21
 C      -3.899076     2.255679    -3.361709      53.42
 H      -3.860407     2.375359    -4.505134      17.79
 C      -4.100954     1.268301    -1.104390      38.87
 C      -4.493584     0.032509    -0.175825     101.29
 H      -5.150194    -0.607170    -0.713188      24.82
 O      -5.350144     0.300199     0.980545     195.45
 H      -4.771262     0.451829     1.768604      24.92
 C      -3.267119    -0.902771     0.029933      85.30
 H      -2.560635    -1.096657    -0.957294      20.66
 C      -3.674825    -2.356034     0.274486     110.60
 O      -4.449959    -3.098489    -0.815829     127.63
 H      -3.933687    -3.355746    -1.707978      25.56
 H      -4.526163    -2.488947     1.103406      24.85
 H      -2.988467    -2.989753     0.642781      26.89
 C       1.075468    -1.102430    -0.468586      57.25
 H       1.251920    -1.524998    -1.535375      16.97
 C       1.236238     0.538068     1.272726      57.18
 H       1.934816     1.185905     1.645465      18.46
 C      -0.177247     0.445691     1.561692      16.41
 O      -0.749623     1.066868     2.681820     223.79
 C      -0.245335     2.293641     3.122492      97.46
 H      -0.950510     3.225426     2.848724      20.98
 H      -0.470467     2.488478     4.381288      22.16
 H       0.693254     2.623567     2.583519      23.33
 C      -1.011676    -0.362794     0.827294       7.28
 O      -2.365445    -0.462056     1.006493     207.02
 C      -0.353204    -1.193300    -0.175442      64.40
 H      -1.035590    -1.822960    -0.792666      20.10
 C       1.869649    -0.109458     0.024294      40.41
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 C       3.340552    -0.161630    -0.265932      95.07
 H       3.632675    -0.484545    -1.310005      24.54
 O       3.687016     1.286075    -0.370451     160.04
 H       3.955379     1.629455     0.578662      23.31
 C       4.438292    -0.746582     0.678287      77.34
 H       4.436420    -0.235453     1.631876      26.53
 O       4.102610    -2.302559     0.818327     246.45
 H       3.760591    -2.723482    -0.029877      27.95
 C       5.881095    -0.836172     0.141909     102.95
 O       6.470713     0.591993     0.118528     189.74
 H       6.609918     1.048371     1.007470      28.87
 H       5.915738    -0.984025    -0.945576      29.96
 H       6.527013    -1.479520     0.697999      31.54
55
name= lig-ACN-Water-frame_671
 C      -4.274953     1.182235    -2.528364      38.13
 H      -4.721889     0.143049    -2.886913      22.43
 C      -3.486852     2.393404    -0.583273      64.98
 H      -3.252430     2.320892     0.378973      17.83
 C      -3.147916     3.529546    -1.344137       9.19
 O      -2.783695     4.835500    -0.730935     255.82
 C      -2.180359     4.879373     0.604643     120.50
 H      -1.234426     4.370801     0.977020      25.86
 H      -2.744312     4.366629     1.215717      30.60
 H      -2.240996     5.980800     0.822654      22.38
 C      -3.355544     3.513745    -2.748917       6.01
 O      -3.170560     4.675359    -3.652409     141.11
 H      -2.658391     5.615449    -3.421237      18.51
 C      -3.864097     2.340650    -3.365834      58.20
 H      -4.122993     1.948956    -4.413432      16.64
 C      -4.056807     1.209199    -1.180679      18.49
 C      -4.523958     0.023849    -0.356904      36.64
 H      -5.195668    -0.511889    -1.070747      22.75
 O      -5.405120     0.374813     0.956261      96.05
 H      -4.774308     0.483260     1.723901      21.78
 C      -3.275341    -1.004166    -0.065724      38.26
 H      -2.840891    -0.797606    -1.183739      22.03
 C      -3.753424    -2.517952     0.309058     116.03
 O      -4.502634    -3.105122    -0.811139     146.87
 H      -3.571068    -3.082976    -1.471308      24.20
 H      -4.358715    -2.306156     1.324563      23.20
 H      -2.845210    -2.962790     0.422973      24.77
 C       0.940043    -1.063762    -0.576383      52.96
 H       1.321259    -1.763625    -1.429716      20.55
 C       1.293158     0.624266     1.195090      63.69
 H       1.756527     1.187279     2.028537      18.16
 C      -0.078611     0.508399     1.602511       4.87
 O      -0.722977     0.991717     2.715146     224.66
 C      -0.345812     2.365270     3.192922      90.39
 H      -1.104970     3.080840     2.754281      21.64
 H      -0.177444     2.114241     4.477657      21.26
 H       0.754656     2.498304     3.087640      23.47
 C      -0.923680    -0.289667     0.689905      20.81
 O      -2.292080    -0.450806     1.031416     115.92
 C      -0.354360    -1.140865    -0.115625      62.45
 H      -0.913820    -1.867978    -0.665923      21.25
 C       1.800771    -0.137183     0.160342      30.20
 C       3.304011    -0.137246    -0.224041      83.57
 H       3.234580    -0.721253    -1.168309      22.93
 O       3.611008     1.315248    -0.463024     215.89
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 H       4.068808     1.616113     0.381152      24.79
 C       4.372143    -0.874260     0.603150     120.50
 H       4.289274    -0.573832     1.599233      26.82
 O       4.143211    -2.253135     0.817823     283.07
 H       4.075047    -2.579747    -0.145468      28.23
 C       5.832276    -0.789713     0.170893     106.84
 O       6.531149     0.523392     0.140270     219.56
 H       6.817847     0.769129     1.052889      27.97
 H       5.924571    -1.296322    -0.807750      32.66
 H       6.194245    -1.484714     0.938107      31.72
55
name= lig-ACN-Water-frame_672
 C      -4.328643     1.275690    -2.578311      42.21
 H      -5.010448     0.560994    -3.284895      21.99
 C      -3.470163     2.395481    -0.525587      65.73
 H      -3.456812     2.493974     0.501928      19.41
 C      -3.060025     3.539829    -1.274841       4.32
 O      -2.761927     4.779247    -0.649738     276.49
 C      -2.259616     4.919463     0.719378     129.44
 H      -1.209591     4.518977     0.475618      23.19
 H      -2.876463     4.619466     1.429501      29.75
 H      -2.081484     5.986036     0.991358      24.82
 C      -3.336464     3.551541    -2.767801     -10.24
 O      -3.184007     4.618306    -3.583362     169.97
 H      -2.919267     5.320975    -2.896178      22.18
 C      -3.864496     2.335741    -3.298661      50.69
 H      -3.823803     2.704263    -4.364821      18.93
 C      -4.044479     1.235228    -1.133935      18.15
 C      -4.520611     0.008551    -0.336936      76.69
 H      -5.293577    -0.607413    -0.940735      22.49
 O      -5.373713     0.382122     0.763414     172.87
 H      -4.797999     0.567825     1.602378      24.20
 C      -3.354532    -1.021516    -0.114910      55.82
 H      -2.617163    -1.313404    -0.981982      20.12
 C      -3.716557    -2.495714     0.302521     116.51
 O      -4.496223    -3.063748    -0.771039     233.33
 H      -3.944283    -3.447826    -1.612056      26.75
 H      -4.454519    -2.742864     1.238425      23.03
 H      -2.957963    -3.180402     0.555410      25.41
 C       0.968205    -0.975117    -0.616049      43.66
 H       1.570310    -1.794793    -1.079303      21.04
 C       1.283363     0.708454     1.265568      83.34
 H       2.263240     1.166391     1.741817      16.32
 C      -0.080612     0.564097     1.531657       8.55
 O      -0.681563     0.978132     2.755151     219.11
 C      -0.354672     2.306481     3.306231      90.61
 H      -1.057264     3.080496     2.992902      24.10
 H      -0.817291     2.343245     4.526328      21.72
 H       0.593017     2.760676     2.981502      25.38
 C      -0.926491    -0.246997     0.742960     -17.19
 O      -2.360496    -0.434978     1.023499      69.94
 C      -0.385407    -1.225907    -0.320966      40.09
 H      -0.986233    -2.042974    -0.559998      17.19
 C       1.780627    -0.287513     0.262240      47.55
 C       3.191526    -0.066181    -0.321322      90.10
 H       3.388405    -0.399591    -1.336943      23.27
 O       3.599728     1.323105    -0.526649     243.58
 H       4.045885     1.643056     0.233886      28.78
 C       4.278967    -0.837369     0.717808     103.32
 H       4.217921    -0.429470     1.688844      26.88
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 O       4.106617    -2.320972     0.735484     291.59
 H       4.482014    -2.697368    -0.067939      30.42
 C       5.861626    -0.767289     0.204781     113.90
 O       6.566917     0.441732     0.197718     232.63
 H       6.960885     0.643641     1.106303      28.22
 H       6.031936    -1.230462    -0.791742      32.03
 H       6.491128    -1.353096     0.911187      29.95
55
name= lig-ACN-Water-frame_673
 C      -4.318931     1.382078    -2.556124      31.16
 H      -4.886408     0.401140    -3.032482      19.58
 C      -3.447796     2.384264    -0.505401      56.46
 H      -3.433525     2.392525     0.600955      21.84
 C      -3.090805     3.556219    -1.214646      23.75
 O      -2.779365     4.761812    -0.662618     258.67
 C      -2.274564     4.913750     0.773504     107.93
 H      -1.282148     4.400008     1.086577      25.10
 H      -2.791217     4.503925     1.530775      27.88
 H      -2.226170     5.997216     0.623870      23.44
 C      -3.271426     3.535014    -2.557793      23.99
 O      -3.208389     4.552625    -3.476414     205.50
 H      -2.671679     5.378724    -3.380268      22.51
 C      -3.850084     2.476459    -3.327756      39.97
 H      -4.144927     2.307754    -4.312652      14.17
 C      -4.095565     1.278153    -1.189619      13.94
 C      -4.459830    -0.027881    -0.392997      77.67
 H      -5.057624    -0.648877    -1.216621      24.15
 O      -5.344498     0.358943     0.653113     171.86
 H      -4.867304     0.636991     1.493213      24.92
 C      -3.300294    -1.033016     0.019840      87.11
 H      -2.876862    -0.897175    -1.043016      25.40
 C      -3.713706    -2.477554     0.316656     113.09
 O      -4.533876    -3.049180    -0.789717     236.81
 H      -3.878100    -3.433944    -1.285098      32.32
 H      -4.403941    -2.282143     1.290646      23.55
 H      -2.703891    -2.889930     0.519896      25.30
 C       1.000493    -1.118943    -0.540098      36.83
 H       1.305817    -1.521904    -1.505277      19.33
 C       1.302556     0.568236     1.253341      54.67
 H       1.744804     1.537816     1.852132      16.61
 C      -0.146738     0.606801     1.538758      -9.27
 O      -0.636401     1.005514     2.785067     201.53
 C      -0.443166     2.303345     3.343258      98.33
 H      -1.070584     2.901320     2.816216      25.90
 H      -0.574781     2.181227     4.665231      22.05
 H       0.668655     2.475658     3.465113      23.80
 C      -1.068186    -0.439074     0.651974      -4.44
 O      -2.419281    -0.402101     0.975545     139.33
 C      -0.450573    -1.111207    -0.345084      76.90
 H      -0.886331    -1.869652    -0.931580      23.36
 C       1.832902    -0.137460     0.191388      25.21
 C       3.277464    -0.098997    -0.286308      87.69
 H       3.163242    -0.645586    -1.196089      24.17
 O       3.594753     1.342157    -0.543719     211.62
 H       3.796344     1.718273     0.375381      25.47
 C       4.332756    -0.756282     0.647235      94.73
 H       4.023349    -0.594306     1.666318      26.32
 O       4.023891    -2.381690     0.667919     210.60
 H       4.401836    -2.618576    -0.219999      27.97
 C       5.832786    -0.851164     0.328772      92.31
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 O       6.627054     0.479381     0.262427     221.15
 H       6.821389     0.898220     1.192778      26.63
 H       5.712803    -1.000191    -0.769323      30.10
 H       6.178650    -1.768747     0.846285      30.20
55
name= lig-ACN-Water-frame_674
 C      -4.298521     1.361167    -2.528891      44.85
 H      -4.678725     0.413612    -3.150165      23.87
 C      -3.479185     2.319448    -0.440381      62.16
 H      -3.114376     2.158256     0.672615      17.35
 C      -3.160778     3.520783    -1.097489      11.45
 O      -2.736653     4.774167    -0.590723     297.53
 C      -2.318852     4.920303     0.744981     147.23
 H      -1.310654     4.392959     0.870927      24.41
 H      -3.171382     4.712845     1.209134      29.49
 H      -2.177271     5.930122     1.115999      23.14
 C      -3.306532     3.504830    -2.630138       5.16
 O      -3.167448     4.628741    -3.438960     258.13
 H      -2.504466     5.186375    -2.972263      25.70
 C      -3.909041     2.464814    -3.243332      50.33
 H      -3.907535     2.734666    -4.204870      19.78
 C      -4.039621     1.279638    -1.140350      48.22
 C      -4.405875     0.014530    -0.509304      79.61
 H      -5.075633    -0.738481    -1.207955      22.78
 O      -5.409059     0.308960     0.647814     137.48
 H      -4.855688     0.486466     1.393714      27.25
 C      -3.281638    -0.895089    -0.092813      95.28
 H      -2.598813    -1.156089    -0.925780      23.26
 C      -3.750398    -2.370717     0.358068     112.42
 O      -4.498085    -3.036111    -0.747974     213.76
 H      -3.898853    -3.285002    -1.434974      31.07
 H      -4.339188    -2.577648     1.365990      25.00
 H      -2.980574    -3.209055     0.469120      24.49
 C       0.970257    -1.081709    -0.465178      44.45
 H       1.356207    -1.571147    -1.326873      17.07
 C       1.121244     0.526147     1.221012      65.08
 H       1.851560     1.152353     1.943372      18.00
 C      -0.223087     0.366791     1.478764      26.93
 O      -0.668630     0.941492     2.755861     205.93
 C      -0.408015     2.300830     3.380651      99.11
 H      -0.774440     3.209201     3.036087      25.30
 H      -1.183391     2.040096     4.390414      20.82
 H       0.650369     2.620767     3.471250      23.89
 C      -1.051388    -0.364864     0.774183      16.97
 O      -2.452421    -0.373852     0.966692     162.52
 C      -0.404017    -1.090662    -0.359957      66.90
 H      -1.015151    -1.333648    -1.204609      20.17
 C       1.810996    -0.149194     0.074215      38.59
 C       3.374891    -0.089037    -0.272291      84.99
 H       3.673309    -0.466565    -1.225355      24.52
 O       3.615586     1.339661    -0.519085     205.45
 H       3.762884     1.796846     0.417526      22.43
 C       4.292047    -0.924063     0.688173      77.54
 H       4.279821    -0.506699     1.733861      23.40
 O       3.957499    -2.296728     0.563036     317.43
 H       3.894710    -2.656065    -0.397037      27.09
 C       5.808789    -0.754540     0.297550     106.91
 O       6.621261     0.429180     0.365677     273.46
 H       6.812316     0.751198     1.308050      27.95
 H       6.070759    -1.251543    -0.683903      29.39
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 H       6.406188    -1.384755     1.032082      27.69
55
name= lig-ACN-Water-frame_675
 C      -4.276413     1.253910    -2.546132      32.94
 H      -4.810391     0.394521    -3.086943      20.78
 C      -3.429655     2.366586    -0.354054      47.80
 H      -3.208766     2.163545     0.851438      15.51
 C      -3.185855     3.576901    -1.142895      10.57
 O      -2.697401     4.781172    -0.654993     284.58
 C      -2.425563     4.879760     0.814086      50.06
 H      -1.635416     4.130360     1.104055      26.46
 H      -2.981822     4.514412     1.547454      26.46
 H      -2.030779     5.894386     0.778759      21.30
 C      -3.392722     3.637612    -2.512405       8.16
 O      -3.074955     4.661414    -3.365769     267.01
 H      -2.668939     5.520625    -3.075290      21.16
 C      -3.947705     2.440213    -3.262936      72.48
 H      -4.080939     2.360685    -4.274270      18.40
 C      -4.003984     1.242313    -1.163329       4.26
 C      -4.500816    -0.019578    -0.446450      49.09
 H      -5.199691    -0.528735    -1.368264      22.41
 O      -5.422467     0.206735     0.610247     127.56
 H      -5.030214     0.279410     1.532503      23.67
 C      -3.287339    -0.972940    -0.155198      71.69
 H      -2.787424    -1.040661    -1.094059      24.63
 C      -3.756706    -2.345554     0.320127     117.33
 O      -4.489427    -3.002091    -0.708468     178.13
 H      -3.723602    -3.145077    -1.509550      24.26
 H      -4.548714    -2.099293     1.086131      25.41
 H      -2.722050    -2.636952     0.833340      22.77
 C       0.977894    -1.045543    -0.653005      39.33
 H       1.333862    -1.917260    -1.115549      20.65
 C       1.164233     0.506687     1.123228      82.24
 H       1.815058     0.947403     1.959951      19.55
 C      -0.149752     0.327943     1.680374       1.33
 O      -0.771489     0.891619     2.717029     208.54
 C      -0.382844     2.233293     3.347094      30.71
 H      -0.732116     2.740941     2.547540      23.16
 H      -1.043857     2.373653     4.454237      19.50
 H       0.647644     2.159463     3.800439      22.71
 C      -1.099792    -0.401018     0.682307      16.42
 O      -2.440484    -0.306330     0.982151     139.25
 C      -0.473605    -1.041929    -0.306590      64.90
 H      -1.010693    -1.683738    -1.060246      20.25
 C       1.812941    -0.221359     0.155749      33.76
 C       3.303557    -0.035905    -0.282228      70.05
 H       3.283539    -0.500764    -1.257962      23.24
 O       3.698728     1.381926    -0.417947     225.04
 H       4.037767     1.666418     0.520950      22.13
 C       4.311425    -0.899832     0.695722      80.99
 H       4.057055    -0.890943     1.826179      21.46
 O       3.854737    -2.253928     0.493481     347.94
 H       4.093412    -2.420973    -0.492489      25.13
 C       5.930928    -0.830398     0.337447      94.12
 O       6.566564     0.462168     0.393937     313.60
 H       6.846700     0.755920     1.305440      28.11
 H       6.105126    -1.249560    -0.705131      31.65
 H       6.191688    -1.593875     1.143042      28.80
55
name= lig-ACN-Water-frame_676
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 C      -4.202810     1.302542    -2.488555      44.42
 H      -4.675456     0.456860    -2.938848      22.78
 C      -3.451238     2.383372    -0.514592      72.93
 H      -3.417322     2.541434     0.713807      18.94
 C      -3.205105     3.585046    -1.129254      14.90
 O      -2.697978     4.769387    -0.630313     251.59
 C      -2.433136     4.802646     0.843463     111.71
 H      -1.583758     4.163260     1.064721      23.03
 H      -3.389294     4.905071     1.172054      27.78
 H      -2.131350     5.826652     1.073108      23.75
 C      -3.518553     3.607541    -2.568032     -11.59
 O      -3.021586     4.666360    -3.346019      35.34
 H      -2.546549     5.333407    -2.789811      13.99
 C      -3.952917     2.466558    -3.233944      65.49
 H      -4.106511     2.588391    -4.309241      20.25
 C      -4.003715     1.273717    -1.095232      44.93
 C      -4.509103    -0.047424    -0.423977      72.09
 H      -5.142306    -0.761194    -1.261215      22.60
 O      -5.467652     0.101887     0.651994     121.79
 H      -4.865677     0.302342     1.470374      23.12
 C      -3.342912    -0.914536    -0.150554      96.07
 H      -2.774397    -0.911043    -0.991230      25.79
 C      -3.755068    -2.270697     0.372323     118.82
 O      -4.435036    -3.010767    -0.714530     187.05
 H      -3.686370    -3.425091    -1.460102      22.79
 H      -4.517102    -2.089036     1.162521      25.37
 H      -3.151063    -3.203845     0.802657      22.66
 C       0.891836    -1.057146    -0.703355     -15.80
 H       1.289676    -1.554976    -1.608499      18.43
 C       1.259720     0.509941     1.319628      92.96
 H       1.835757     1.333440     1.646006      16.50
 C      -0.151840     0.304553     1.609063      -1.87
 O      -0.908970     0.847544     2.803718     209.56
 C      -0.337740     2.059224     3.231120     115.87
 H      -0.071568     2.959914     2.609996      25.30
 H      -1.143729     2.491410     4.024032      22.21
 H       0.717360     1.960980     3.537857      25.32
 C      -0.995930    -0.333715     0.751639       3.40
 O      -2.473053    -0.309502     0.881337     113.96
 C      -0.443965    -1.128333    -0.430743      94.40
 H      -1.047796    -2.066784    -0.645458      19.15
 C       1.782186    -0.274889     0.131413      53.71
 C       3.265750    -0.009041    -0.212840      85.23
 H       3.488191    -0.363711    -1.239713      20.52
 O       3.768689     1.400928    -0.345201     198.21
 H       3.973579     1.779824     0.637552      20.13
 C       4.318175    -0.818811     0.599561      98.98
 H       4.177050    -0.309386     1.654340      23.56
 O       3.774515    -2.275412     0.401742     278.89
 H       4.319491    -2.753088    -0.252757      30.26
 C       5.882214    -0.944628     0.466098      99.86
 O       6.523165     0.487766     0.350552     281.26
 H       6.710242     0.941749     1.240141      28.76
 H       6.006260    -1.239706    -0.614083      31.38
 H       6.575837    -1.659102     1.034543      30.05
55
name= lig-ACN-Water-frame_677
 C      -4.207081     1.335087    -2.497146      46.45
 H      -4.410600     0.508714    -3.045327      26.16
 C      -3.531023     2.439523    -0.455937      49.26
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 H      -3.317996     2.299127     0.721839      19.57
 C      -3.249366     3.607613    -1.229360      15.58
 O      -2.658142     4.749950    -0.597121     300.07
 C      -2.518066     4.815292     0.811104      95.39
 H      -2.130621     3.938391     1.297627      25.76
 H      -3.337652     4.527762     1.424647      23.44
 H      -1.932666     5.713431     1.065157      23.63
 C      -3.431661     3.672369    -2.621615      13.18
 O      -3.022492     4.647981    -3.351648     117.44
 H      -2.813318     5.539714    -2.833630      19.97
 C      -3.987549     2.489892    -3.231988      72.32
 H      -4.012793     2.524753    -4.408264      20.79
 C      -4.101555     1.261611    -1.090140      37.71
 C      -4.485970     0.006583    -0.449663      71.18
 H      -5.121921    -0.637640    -1.335026      22.63
 O      -5.443072     0.072264     0.740282     105.06
 H      -5.062623     0.490261     1.526116      25.99
 C      -3.216129    -0.896279    -0.100784      87.32
 H      -2.839196    -1.179887    -0.972814      26.21
 C      -3.840590    -2.392245     0.412029     100.54
 O      -4.416566    -3.032321    -0.748820     236.55
 H      -3.679465    -3.430289    -1.254527      28.20
 H      -4.573571    -2.377762     1.159372      25.43
 H      -2.709139    -2.688984     0.792458      22.64
 C       0.932781    -1.014502    -0.652484      65.77
 H       1.367135    -1.360493    -1.648649      15.67
 C       1.235651     0.388816     1.359815      66.79
 H       1.782357     1.085285     1.816032      17.84
 C      -0.229908     0.357600     1.608265       8.89
 O      -0.935875     0.777323     2.720792     182.29
 C      -0.214993     2.020659     3.202052      91.69
 H      -0.132352     2.560245     2.178829      20.90
 H      -0.844225     2.520164     4.019150      23.19
 H       0.575419     1.553802     3.829120      23.59
 C      -1.015922    -0.441743     0.622344      23.08
 O      -2.369117    -0.281203     0.846827     186.05
 C      -0.479734    -1.205239    -0.345849      69.13
 H      -1.113367    -1.801201    -1.095598      18.97
 C       1.741505    -0.155311     0.173460      11.26
 C       3.400949     0.017017    -0.328518      55.81
 H       3.368808    -0.334161    -1.422007      22.96
 O       3.729188     1.392438    -0.373605     231.20
 H       3.889481     1.696662     0.606655      21.46
 C       4.253903    -0.925831     0.631605      70.60
 H       4.036780    -0.852556     1.799487      23.22
 O       3.744983    -2.211147     0.470948     347.05
 H       3.926882    -2.500813    -0.471068      27.76
 C       5.823752    -0.812906     0.362373     101.75
 O       6.458750     0.402056     0.282369     309.08
 H       6.759448     0.663888     1.227619      27.27
 H       6.180216    -1.480220    -0.445449      31.16
 H       6.049353    -1.279073     1.428763      26.44
55
name= lig-ACN-Water-frame_678
 C      -4.283776     1.326024    -2.564026      42.18
 H      -4.548715     0.475892    -3.015229      23.92
 C      -3.662151     2.472444    -0.401128      63.29
 H      -3.330568     2.454738     0.667767      16.58
 C      -3.248766     3.604278    -1.118771      13.87
 O      -2.643477     4.720929    -0.647359     216.46
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 C      -2.618687     4.711247     0.895005     110.82
 H      -1.907938     3.978901     1.038594      24.60
 H      -3.563859     5.120179     1.256877      25.02
 H      -2.024487     5.645821     0.992169      22.96
 C      -3.378618     3.617419    -2.569028       1.61
 O      -3.016340     4.777014    -3.476546     222.92
 H      -2.656537     5.651104    -2.936232      21.90
 C      -3.944852     2.540402    -3.283815      54.40
 H      -3.962003     2.334034    -4.477556      18.52
 C      -4.165748     1.383823    -1.147185      32.50
 C      -4.444031    -0.016433    -0.328564      82.47
 H      -5.171897    -0.670530    -1.115953      22.23
 O      -5.354429     0.119734     0.764498     191.60
 H      -4.792373     0.408863     1.502799      25.51
 C      -3.351983    -1.028896    -0.059839      91.90
 H      -2.804559    -1.043264    -0.896500      24.80
 C      -3.759084    -2.386194     0.391958     127.21
 O      -4.389737    -3.084556    -0.746848     263.57
 H      -3.788528    -3.270344    -1.362812      32.26
 H      -4.481481    -2.284197     1.112118      26.43
 H      -2.957105    -3.251223     0.821999      22.90
 C       0.971421    -0.942143    -0.586375      74.45
 H       1.428895    -1.670483    -1.355204      21.19
 C       1.123477     0.363211     1.368436      85.08
 H       1.616251     0.403811     2.212666      19.79
 C      -0.229224     0.207114     1.503673       6.95
 O      -0.914598     0.784316     2.605026     171.10
 C      -0.153339     1.933273     3.256862      95.53
 H       0.440733     2.639368     2.369836      20.77
 H      -0.855560     2.572526     3.726734      24.12
 H       0.829224     1.727707     3.711490      23.75
 C      -1.004600    -0.487827     0.630354      17.67
 O      -2.347674    -0.266989     0.831903     131.40
 C      -0.359897    -1.249833    -0.374569      72.35
 H      -0.872912    -1.540928    -1.324708      16.68
 C       1.842788    -0.111242     0.112348      26.73
 C       3.270532    -0.001121    -0.320162      84.60
 H       3.461050    -0.535539    -1.350530      23.54
 O       3.683668     1.414645    -0.453882     214.38
 H       3.996818     1.800116     0.416339      23.31
 C       4.151969    -0.868428     0.587917      86.61
 H       3.953742    -0.367423     1.652008      21.53
 O       3.730656    -2.262320     0.539804     280.38
 H       3.615520    -2.509503    -0.453203      26.74
 C       5.720595    -0.886863     0.419392      93.83
 O       6.444764     0.425917     0.182386     267.05
 H       6.837894     0.815574     1.042151      27.18
 H       5.990968    -1.585780    -0.411004      30.77
 H       6.273099    -1.373944     1.373364      27.59
55
name= lig-ACN-Water-frame_681
 C      -4.358124     1.329685    -2.602380      31.13
 H      -4.636244     0.377371    -3.205774      23.73
 C      -3.842946     2.529586    -0.535318      74.74
 H      -3.719366     2.413801     0.508876      20.22
 C      -3.273848     3.646043    -1.180045      12.93
 O      -2.690285     4.670320    -0.620580     170.39
 C      -2.740199     4.841719     0.926753      91.40
 H      -2.444477     4.018852     1.578243      26.30
 H      -3.851589     4.597860     1.356438      24.68
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 H      -2.088153     5.731415     1.191631      23.79
 C      -3.334560     3.549763    -2.684575     -26.11
 O      -3.056817     4.700209    -3.529619     197.91
 H      -2.407655     5.319371    -3.148527      21.20
 C      -3.912815     2.481537    -3.290849      60.73
 H      -3.678214     2.709470    -4.326424      22.95
 C      -4.331029     1.371151    -1.170431       4.61
 C      -4.651363     0.058292    -0.345470      72.77
 H      -5.376107    -0.575118    -1.061274      23.19
 O      -5.341294     0.308882     0.820859     228.40
 H      -4.752648     0.475574     1.658981      21.68
 C      -3.436043    -1.018908    -0.298355      54.94
 H      -3.257109    -1.119309    -1.427130      26.47
 C      -3.673952    -2.399830     0.208148     118.25
 O      -4.487205    -3.304182    -0.674471     140.41
 H      -3.735305    -3.714130    -1.426804      24.38
 H      -4.247167    -2.151538     1.138987      25.68
 H      -2.753383    -3.039471     0.519931      24.93
 C       0.952409    -1.032634    -0.822522      61.90
 H       1.301299    -1.606135    -1.658472      27.34
 C       1.286944     0.265010     1.169257      57.44
 H       1.924164     0.906940     1.895307      18.55
 C      -0.073854     0.153327     1.420229       1.68
 O      -0.865487     0.960091     2.484816     132.05
 C      -0.019002     1.784440     3.403351     100.22
 H       0.618062     2.670582     2.678967      21.25
 H      -0.800801     2.281702     3.857216      26.21
 H       0.488650     1.144065     4.196793      25.52
 C      -0.917559    -0.588533     0.549772      15.76
 O      -2.271144    -0.557533     0.795038      55.78
 C      -0.393225    -1.308086    -0.518599      84.56
 H      -1.142617    -1.471407    -1.262391      19.71
 C       1.829903    -0.338225    -0.003960      41.06
 C       3.314340    -0.080538    -0.247333      74.13
 H       3.529234    -0.230897    -1.416698      21.31
 O       3.492468     1.526001    -0.545180     125.37
 H       4.044370     1.874329     0.227140      24.43
 C       4.219977    -0.727207     0.721513     108.15
 H       4.163614    -0.291824     1.809043      23.99
 O       3.788971    -2.139394     0.742744     299.39
 H       4.014006    -2.462281    -0.136399      28.91
 C       5.681556    -0.863568     0.334920     103.11
 O       6.340361     0.472545    -0.008782     238.42
 H       6.717282     0.696830     0.911738      28.72
 H       5.742751    -1.319307    -0.713153      30.24
 H       6.300323    -1.411106     1.091070      28.94
55
name= lig-ACN-Water-frame_682
 C      -4.344503     1.254442    -2.648224     -30.07
 H      -4.620240     0.191216    -3.152891      16.56
 C      -3.809019     2.483109    -0.445402      41.39
 H      -3.668979     2.471107     0.696586      18.47
 C      -3.329933     3.554815    -1.249237      -2.86
 O      -2.712655     4.755956    -0.553113     202.74
 C      -2.777283     4.819037     0.887973      97.07
 H      -2.119619     4.051631     1.302123      25.03
 H      -3.962533     5.104807     1.014412      24.51
 H      -2.483532     5.901150     1.121427      23.79
 C      -3.378670     3.616961    -2.650654      -2.88
 O      -3.003136     4.595251    -3.522838     156.10
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 H      -2.666624     5.440751    -2.990766      21.70
 C      -3.934311     2.429966    -3.397549      33.29
 H      -4.100668     2.369663    -4.411229      22.68
 C      -4.371096     1.358645    -1.208252     -21.50
 C      -4.605303     0.116366    -0.405976      81.51
 H      -5.348534    -0.514155    -1.091040      21.24
 O      -5.440547     0.306558     0.817188     177.51
 H      -4.807356     0.280575     1.570976      25.63
 C      -3.388211    -0.903968    -0.335688      52.85
 H      -2.754216    -0.831448    -1.348246      24.04
 C      -3.727829    -2.451999     0.180328      99.84
 O      -4.543985    -3.357998    -0.638256     193.40
 H      -3.988507    -3.513217    -1.493292      28.32
 H      -4.380420    -2.567501     1.136184      24.01
 H      -2.690858    -2.752779     0.402816      26.02
 C       0.983393    -1.151063    -0.932520       7.88
 H       1.380580    -1.442872    -1.855969      19.14
 C       1.263832     0.331403     1.002067      88.83
 H       2.098286     0.369878     1.843622      17.43
 C      -0.138406     0.243616     1.402780      14.11
 O      -0.795624     0.954405     2.429197     178.06
 C      -0.080321     1.732102     3.437885     102.02
 H       0.885229     2.554324     3.000020      22.10
 H      -0.727426     2.285876     4.134588      25.23
 H       0.595503     1.009032     3.958196      26.07
 C      -0.950917    -0.622081     0.556134      21.93
 O      -2.335510    -0.595858     0.741756     158.24
 C      -0.405095    -1.232478    -0.565905      62.97
 H      -0.963282    -1.765969    -1.363448      21.60
 C       1.849444    -0.361257    -0.050427      33.56
 C       3.307550    -0.047274    -0.383195      60.28
 H       3.606449    -0.774256    -1.314589      21.54
 O       3.440900     1.492476    -0.417679     124.95
 H       4.041863     1.735842     0.313806      24.13
 C       4.340883    -0.642639     0.715312     105.71
 H       4.090088    -0.223875     1.731548      25.65
 O       3.843622    -2.135289     0.810338     265.76
 H       3.750278    -2.509840    -0.130563      27.93
 C       5.779645    -0.863599     0.269564      94.38
 O       6.358996     0.568959    -0.008305     217.51
 H       6.725990     1.024888     0.803344      29.28
 H       5.738569    -1.392940    -0.715728      32.63
 H       6.219384    -1.611969     0.945999      31.39
55
name= lig-ACN-Water-frame_683
 C      -4.313830     1.347927    -2.560078      77.96
 H      -4.799647     0.428359    -3.189064      25.44
 C      -3.788510     2.433193    -0.556231      75.75
 H      -3.937621     2.449321     0.648736      19.84
 C      -3.324987     3.609075    -1.189411      -4.48
 O      -2.758237     4.751261    -0.652404     195.43
 C      -2.885275     4.900383     0.813266      86.42
 H      -2.282286     4.129929     1.382034      24.60
 H      -3.837598     4.566708     1.566122      23.01
 H      -2.267101     5.804054     1.008091      24.81
 C      -3.522693     3.506778    -2.721829     -43.00
 O      -2.916293     4.558664    -3.468565      57.29
 H      -2.913751     5.438365    -2.913649      20.69
 C      -3.950298     2.370966    -3.359433      79.21
 H      -4.049886     2.377561    -4.350392      18.07
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 C      -4.271120     1.331663    -1.192538      45.08
 C      -4.629638     0.025486    -0.467427      61.31
 H      -5.285576    -0.665474    -1.138188      24.83
 O      -5.455890     0.260587     0.804797     156.31
 H      -4.867451     0.400484     1.557584      26.94
 C      -3.335012    -0.915876    -0.259945      73.04
 H      -2.802195    -0.934822    -1.380307      24.89
 C      -3.771859    -2.449101     0.140958     108.65
 O      -4.589397    -3.343656    -0.642821     255.46
 H      -4.054677    -3.467754    -1.345469      34.81
 H      -4.118628    -2.160456     1.270634      24.56
 H      -2.909488    -3.014409     0.252443      26.46
 C       1.048766    -1.147724    -0.987256      17.62
 H       1.303848    -1.666305    -1.861660      19.70
 C       1.204573     0.293927     1.058993      65.94
 H       1.712920     1.255190     1.662124      14.96
 C      -0.136746     0.279363     1.291990      13.04
 O      -0.739157     0.954689     2.356467     182.56
 C      -0.019596     1.603382     3.465485      85.20
 H       0.575536     2.606764     2.797501      19.64
 H      -0.980696     2.037600     4.013762      22.35
 H       0.572643     0.915307     4.131252      24.26
 C      -0.986900    -0.548178     0.472089      -9.85
 O      -2.479586    -0.561537     0.747084     169.53
 C      -0.340218    -1.200863    -0.705968     106.49
 H      -0.979919    -2.091165    -0.973047      22.49
 C       1.810657    -0.362982    -0.186206      29.06
 C       3.333414     0.005303    -0.410879      78.98
 H       3.722873    -0.059423    -1.570779      21.00
 O       3.426389     1.371347    -0.338425     247.49
 H       3.815631     1.671298     0.516033      23.59
 C       4.296331    -0.793090     0.619385      93.07
 H       4.394722    -0.254024     1.561155      25.79
 O       3.910851    -2.065071     0.921849     307.91
 H       4.110958    -2.595031     0.052871      27.91
 C       5.863266    -0.687414     0.159772     113.87
 O       6.408657     0.581178     0.008804     274.41
 H       6.579853     0.793819     0.949100      30.35
 H       6.047322    -1.177452    -0.797561      31.14
 H       6.553290    -0.995484     0.927847      28.51
55
name= lig-ACN-Water-frame_684
 C      -4.398045     1.248795    -2.557817       4.33
 H      -4.870575     0.243194    -3.036392      28.70
 C      -3.770531     2.497506    -0.518143      25.69
 H      -3.691850     2.516679     0.719325      13.44
 C      -3.407386     3.556688    -1.318697      32.22
 O      -2.882002     4.726692    -0.741453     236.72
 C      -2.853156     4.895439     0.807091      74.59
 H      -2.150384     4.122278     1.182142      25.43
 H      -4.126440     4.877565     0.875571      23.36
 H      -2.740386     5.969963     1.076686      24.66
 C      -3.443143     3.592542    -2.648807      32.68
 O      -2.887581     4.538820    -3.408545     166.35
 H      -2.606523     5.274608    -2.815294      22.82
 C      -3.970990     2.450978    -3.323198      41.93
 H      -3.871506     2.474280    -4.403318      21.42
 C      -4.195356     1.212786    -1.142535     -61.24
 C      -4.639783    -0.089831    -0.410631      72.29
 H      -5.382234    -0.559139    -1.110052      21.29
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 O      -5.399694     0.178063     0.729474     198.69
 H      -4.731536     0.419852     1.457225      25.87
 C      -3.455997    -1.078222    -0.307216      64.06
 H      -2.936158    -1.057767    -1.447924      23.17
 C      -3.689433    -2.414363     0.198665     110.63
 O      -4.663538    -3.236493    -0.657910     164.45
 H      -4.147963    -3.684127    -1.333759      31.20
 H      -4.536227    -2.429341     1.104135      22.80
 H      -2.807316    -2.845491     0.461722      26.94
 C       0.987062    -1.110109    -1.010763      59.60
 H       1.566036    -1.817486    -1.583205      23.13
 C       1.253689     0.277804     0.946410      46.91
 H       1.801999     1.386118     1.215807      13.72
 C      -0.186760     0.223295     1.184080       2.85
 O      -0.763197     0.926815     2.296559     151.54
 C      -0.028871     1.510575     3.383618      93.79
 H       0.796902     2.587381     3.361371      20.89
 H      -0.847148     1.868694     4.233474      22.32
 H       0.655704     0.743221     3.852588      24.40
 C      -1.071295    -0.454562     0.274961      21.66
 O      -2.372881    -0.477585     0.763379     138.34
 C      -0.436434    -1.250771    -0.660934      80.14
 H      -0.955780    -1.944629    -1.419932      21.01
 C       1.852995    -0.254256    -0.133692      24.54
 C       3.314087    -0.083415    -0.421011      74.93
 H       3.385438    -0.465205    -1.547872      20.89
 O       3.478542     1.444506    -0.243971     203.74
 H       3.707348     1.686148     0.722149      21.91
 C       4.377389    -0.725851     0.475862      96.16
 H       4.133210    -0.184235     1.350006      26.45
 O       3.979752    -2.118484     0.992615     296.38
 H       4.398231    -2.816730     0.491903      29.99
 C       5.913368    -0.681495     0.087607     101.94
 O       6.461561     0.740454     0.023876     240.10
 H       6.798647     1.129956     0.889106      28.30
 H       6.090252    -1.185627    -0.831218      31.41
 H       6.226746    -1.410655     0.789233      32.20
55
name= lig-ACN-Water-frame_685
 C      -4.397678     1.279121    -2.553581      72.07
 H      -4.676279     0.372738    -3.234087      23.20
 C      -3.796123     2.345512    -0.460110      55.55
 H      -3.418156     2.492349     0.678455      16.44
 C      -3.458454     3.560337    -1.183147     -18.57
 O      -2.948661     4.770200    -0.747566     207.25
 C      -2.963642     4.904193     0.609424     110.37
 H      -2.248910     4.253839     1.282141      24.62
 H      -4.033318     4.599307     1.358473      23.49
 H      -2.473315     5.873861     0.706236      24.62
 C      -3.390359     3.512140    -2.701729     -18.97
 O      -2.827281     4.625138    -3.399770     184.61
 H      -2.460369     5.269473    -2.786070      23.05
 C      -4.043516     2.400556    -3.247665      60.16
 H      -4.301443     2.354735    -4.397487      26.18
 C      -4.199743     1.201702    -1.159982      50.17
 C      -4.602679    -0.103229    -0.473637      96.20
 H      -5.297638    -0.651119    -1.117383      25.79
 O      -5.345259     0.083418     0.774954     167.75
 H      -4.765036     0.347403     1.565790      24.16
 C      -3.471123    -1.094706    -0.305749      63.88
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 H      -2.828945    -1.297177    -1.358429      22.57
 C      -3.792356    -2.533761     0.337448     112.16
 O      -4.656638    -3.115973    -0.667520     123.12
 H      -3.893301    -3.507770    -1.423875      24.10
 H      -4.232818    -2.324270     1.497513      24.05
 H      -2.952697    -3.161047     0.411573      26.39
 C       0.939151    -1.099094    -0.874601      56.37
 H       1.237805    -1.669013    -1.790142      24.85
 C       1.153939     0.477856     0.872421      69.54
 H       1.871729     0.776577     1.903700      17.35
 C      -0.136822     0.268476     1.150606      17.88
 O      -0.814153     0.903085     2.174053     171.92
 C       0.004967     1.376255     3.367215      75.82
 H       0.609367     2.361171     2.748777      20.05
 H      -0.809478     1.608027     4.299295      22.17
 H       0.702688     0.496533     3.646181      24.63
 C      -1.039982    -0.408366     0.244744       5.48
 O      -2.359464    -0.444257     0.597912     130.96
 C      -0.434251    -1.276462    -0.758978      61.30
 H      -1.062185    -1.769593    -1.547963      19.66
 C       1.792666    -0.384828    -0.178044      50.82
 C       3.281990    -0.068440    -0.477247      75.21
 H       3.646039    -0.219628    -1.559792      22.33
 O       3.553033     1.494761    -0.258318      98.77
 H       4.215222     1.609529     0.508907      20.44
 C       4.401833    -0.673808     0.504604     101.72
 H       4.523689    -0.173085     1.388968      25.45
 O       4.090193    -2.142365     1.020983     256.96
 H       4.348293    -2.634490     0.205932      28.30
 C       5.886813    -0.669132     0.046256     106.12
 O       6.491472     0.814415     0.031768     185.17
 H       6.803941     0.788496     1.013440      27.25
 H       5.991762    -0.896842    -0.957762      30.89
 H       6.585587    -1.064126     0.704223      30.95
55
name= lig-ACN-Water-frame_686
 C      -4.382965     1.285678    -2.543690      24.14
 H      -4.839492     0.377627    -3.013690      18.49
 C      -3.735435     2.324072    -0.450372      45.48
 H      -3.835973     2.013069     0.628840      21.26
 C      -3.428864     3.471342    -1.236012      10.27
 O      -3.062288     4.734814    -0.784691     217.57
 C      -2.958356     4.989606     0.665311      81.86
 H      -2.210330     4.142389     0.856042      23.59
 H      -4.217038     4.816800     1.184282      22.05
 H      -2.740202     6.030653     0.955523      23.20
 C      -3.402886     3.486370    -2.628846     -12.00
 O      -2.817283     4.594989    -3.374885     159.54
 H      -2.816718     5.402579    -2.733025      19.22
 C      -4.061229     2.449881    -3.322404      42.14
 H      -4.261927     2.509095    -4.522755      27.55
 C      -4.260788     1.199673    -1.144540      33.12
 C      -4.580372    -0.147485    -0.491063      73.99
 H      -5.263291    -0.612028    -1.103832      26.48
 O      -5.311183    -0.004024     0.848346     173.18
 H      -4.627796     0.207841     1.469481      28.53
 C      -3.295562    -1.163496    -0.201644      86.97
 H      -3.112151    -1.437713    -1.377202      23.71
 C      -3.828800    -2.523508     0.390599     103.20
 O      -4.667275    -3.072942    -0.651389     129.41
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 H      -3.949074    -3.071615    -1.559162      23.29
 H      -4.515753    -2.527967     1.438907      22.91
 H      -2.917071    -3.104810     0.563944      25.69
 C       0.956484    -1.256127    -1.002443      39.74
 H       1.471778    -1.630752    -1.950197      17.91
 C       1.224726     0.490781     0.866602      48.82
 H       1.988724     0.848716     1.873510      13.57
 C      -0.233355     0.375727     1.066170       9.65
 O      -0.889837     0.890663     2.176247     181.57
 C       0.002800     1.199412     3.181519      92.18
 H       0.683189     2.356585     3.164824      20.68
 H      -0.771752     1.552350     4.138340      21.78
 H       0.785137     0.438149     3.569642      23.16
 C      -1.006173    -0.500030     0.247738      19.27
 O      -2.420863    -0.392494     0.435411     197.54
 C      -0.481623    -1.146681    -0.814708      96.15
 H      -1.073884    -1.871842    -1.321648      24.89
 C       1.805748    -0.283432    -0.105032       1.69
 C       3.390060     0.066609    -0.405407      68.57
 H       3.455879    -0.252479    -1.487805      21.75
 O       3.585359     1.440344    -0.392296     241.37
 H       4.116398     1.729743     0.395737      23.25
 C       4.415877    -0.740812     0.665740     104.85
 H       4.158859    -0.235590     1.518283      28.10
 O       4.237304    -2.060439     0.930294     313.25
 H       3.931055    -2.592484     0.116147      27.57
 C       5.909732    -0.496521    -0.010274     105.49
 O       6.445084     0.768720     0.041627     270.86
 H       6.840243     1.092338     0.925762      27.70
 H       5.910054    -1.044645    -0.957287      30.89
 H       6.391062    -1.305805     0.515041      30.90
55
name= lig-ACN-Water-frame_687
 C      -4.448030     1.268508    -2.619546      55.35
 H      -4.960560     0.490081    -3.133871      25.17
 C      -3.735189     2.326240    -0.441875      50.47
 H      -3.724769     2.759388     0.506713      16.48
 C      -3.347847     3.421647    -1.226099     -23.08
 O      -3.165643     4.760511    -0.772311     167.32
 C      -2.978913     4.988017     0.717680     102.10
 H      -2.248874     4.475243     1.492638      22.30
 H      -4.215253     4.766042     1.268513      22.02
 H      -2.653199     6.036182     0.646025      23.72
 C      -3.443865     3.504273    -2.664123       4.26
 O      -2.882809     4.487821    -3.305250     171.94
 H      -2.773635     5.357656    -2.787444      20.92
 C      -4.037217     2.444618    -3.344894      48.39
 H      -4.018071     2.538291    -4.532670      23.15
 C      -4.260672     1.155476    -1.161747     -27.79
 C      -4.591405    -0.230877    -0.391926      90.33
 H      -5.246707    -0.750372    -0.936017      27.49
 O      -5.249919    -0.073149     0.847827     152.23
 H      -4.660055     0.126038     1.623311      24.22
 C      -3.421074    -1.185641    -0.278974      94.18
 H      -2.765721    -1.494537    -1.158106      24.32
 C      -3.788622    -2.477135     0.397533     120.17
 O      -4.677337    -3.085131    -0.635704     158.74
 H      -4.214721    -3.233532    -1.523299      30.83
 H      -4.604523    -2.239133     1.234699      24.07
 H      -3.037348    -3.217465     0.864813      25.75
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 C       1.078960    -1.099787    -1.021884      23.51
 H       1.518654    -1.930689    -1.668523      19.34
 C       1.151332     0.362102     0.917236      90.00
 H       1.653984     1.545547     1.087504      17.01
 C      -0.231513     0.417137     0.997132      10.58
 O      -0.929266     0.877149     2.128494     163.76
 C      -0.014522     1.177004     3.234864      63.18
 H       0.780898     2.111633     2.799115      18.93
 H      -0.656457     1.212581     4.319408      22.21
 H       0.553711     0.155199     3.265566      22.84
 C      -1.041296    -0.460118     0.231649       5.82
 O      -2.354944    -0.280363     0.434035     143.82
 C      -0.345439    -1.205262    -0.912272      62.66
 H      -0.903034    -1.832382    -1.523485      22.04
 C       1.856293    -0.264637    -0.217951      43.70
 C       3.348036    -0.057672    -0.298403      86.76
 H       3.755494    -0.535093    -1.193409      24.31
 O       3.636253     1.454485    -0.503603     190.34
 H       3.696137     1.795734     0.402657      24.92
 C       4.425620    -0.554842     0.660548     112.05
 H       4.496416    -0.235333     1.641276      26.75
 O       4.310705    -2.073328     0.838022     260.02
 H       4.260870    -2.539187    -0.120401      25.56
 C       5.820623    -0.554943     0.121880      99.92
 O       6.437449     0.814073    -0.011198     222.92
 H       6.723599     0.940042     0.907272      29.79
 H       5.616803    -0.564003    -0.972994      30.66
 H       6.613832    -1.143724     0.558370      31.59
55
name= lig-ACN-Water-frame_688
 C      -4.508106     1.250025    -2.579661      79.54
 H      -4.783328     0.444924    -3.161364      31.08
 C      -3.781872     2.332257    -0.503302      56.68
 H      -3.718619     2.069823     0.445140      17.94
 C      -3.368638     3.494775    -1.199587      16.53
 O      -3.175248     4.720761    -0.635874     211.78
 C      -3.059695     5.045168     0.712534      83.26
 H      -2.174352     4.299802     1.014555      24.85
 H      -4.156138     4.981739     1.510306      22.65
 H      -2.808654     6.140098     0.817599      24.54
 C      -3.472027     3.392501    -2.632958      16.20
 O      -2.906561     4.522670    -3.350452     189.95
 H      -2.444387     4.986260    -2.663634      25.32
 C      -4.038037     2.334431    -3.295086      59.41
 H      -4.271990     2.363725    -4.383493      15.87
 C      -4.256494     1.120252    -1.188287     -48.69
 C      -4.632477    -0.210369    -0.467813      78.07
 H      -5.305928    -0.675903    -1.020177      25.37
 O      -5.220624    -0.093266     0.909063     138.16
 H      -4.495850     0.263315     1.527365      24.60
 C      -3.336527    -1.089648    -0.343619      89.61
 H      -3.205967    -1.191742    -1.444023      25.41
 C      -3.866700    -2.443220     0.395500      97.33
 O      -4.681798    -3.156454    -0.599163     246.99
 H      -4.032168    -3.469245    -1.097164      35.52
 H      -4.334050    -2.166114     1.356443      24.10
 H      -2.818964    -3.034067     0.530627      23.13
 C       1.129601    -1.037435    -1.045650      48.32
 H       1.701402    -1.701659    -1.751969      25.53
 C       1.138571     0.444878     0.779034      45.10
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 H       1.680600     1.376810     1.496785      17.38
 C      -0.247119     0.262501     1.011927       6.56
 O      -0.924536     0.938902     2.082779     165.10
 C      -0.017621     1.072929     3.253391      89.25
 H       0.629387     2.242611     3.261901      21.20
 H      -0.758437     1.481849     4.199431      22.26
 H       0.794250     0.302613     3.469739      24.56
 C      -0.971591    -0.427938    -0.006833      15.81
 O      -2.374386    -0.285042     0.451618     182.32
 C      -0.242646    -1.200052    -0.862834      71.89
 H      -0.632442    -1.837870    -1.589099      20.61
 C       1.882116    -0.244057    -0.132850      35.67
 C       3.364833    -0.101979    -0.319041      77.06
 H       3.566373    -0.487319    -1.271797      25.83
 O       3.626770     1.424957    -0.549446     147.01
 H       4.100367     1.795799     0.272971      23.43
 C       4.425348    -0.593797     0.777650     104.52
 H       4.234673    -0.128505     1.750458      25.91
 O       4.309670    -2.059929     0.803983     264.18
 H       4.635904    -2.443693    -0.045664      29.51
 C       5.810145    -0.447997     0.053798     101.92
 O       6.461981     0.858673    -0.023998     198.47
 H       6.822861     1.162765     0.807421      28.32
 H       5.857141    -1.158518    -0.836828      30.20
 H       6.296139    -1.180680     0.761389      29.96
55
name= lig-ACN-Water-frame_689
 C      -4.534936     1.106951    -2.541348      63.17
 H      -4.974445     0.250859    -2.938479      22.86
 C      -3.816457     2.213378    -0.477954      69.96
 H      -3.625235     2.282091     0.462182      24.84
 C      -3.535500     3.447683    -1.144502     -31.06
 O      -3.187870     4.738900    -0.651315     184.37
 C      -3.056366     5.046102     0.821609      85.71
 H      -2.221991     4.480617     1.499026      24.80
 H      -4.239217     4.646954     1.291255      21.60
 H      -2.776316     6.154995     0.817423      22.98
 C      -3.391850     3.466034    -2.611820     -38.03
 O      -2.958153     4.510321    -3.368425     215.53
 H      -2.285327     5.074926    -2.921963      22.62
 C      -4.067175     2.294734    -3.277856      39.14
 H      -4.099170     2.343308    -4.311583      26.20
 C      -4.351005     1.151878    -1.198930      79.31
 C      -4.632695    -0.095617    -0.482592     109.02
 H      -5.316259    -0.656420    -0.981884      27.94
 O      -5.180107    -0.025146     0.919021     152.29
 H      -4.515653     0.275812     1.550006      25.51
 C      -3.408570    -1.015642    -0.397760      93.34
 H      -2.863079    -1.307576    -1.267646      24.41
 C      -3.766712    -2.365325     0.272958     113.14
 O      -4.667731    -3.233339    -0.512396     229.39
 H      -4.181907    -3.686062    -1.274491      30.28
 H      -4.349681    -2.328715     1.115041      25.88
 H      -2.800973    -3.066085     0.641170      23.10
 C       1.222282    -1.074071    -1.025930      39.56
 H       1.691030    -1.413990    -1.953744      22.76
 C       1.156289     0.623071     0.817135      65.55
 H       1.821607     0.743016     1.829756      19.01
 C      -0.184820     0.240940     1.026249       9.45
 O      -0.809331     0.932464     2.060409     175.67
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 C      -0.080868     1.151801     3.283811      97.91
 H       0.658166     2.227718     3.140636      20.79
 H      -0.956348     0.978977     4.099639      22.92
 H       0.476761     0.218192     3.578202      25.65
 C      -1.049451    -0.360388     0.049767       3.24
 O      -2.340533    -0.433288     0.321018     206.69
 C      -0.249022    -1.217021    -0.979709      36.47
 H      -0.893378    -1.937898    -1.492735      18.81
 C       1.898364    -0.222516    -0.100300      17.31
 C       3.394119     0.009312    -0.361168     101.93
 H       3.654631    -0.547759    -1.197840      26.18
 O       3.615806     1.366195    -0.539352     203.84
 H       4.457917     1.611135    -0.029958      20.57
 C       4.352812    -0.678850     0.634309      96.66
 H       4.205729    -0.325490     1.709804      23.03
 O       4.277915    -2.047459     0.893317     314.08
 H       4.128418    -2.546901     0.069730      29.11
 C       5.921264    -0.407807     0.169385      89.61
 O       6.480701     0.891395    -0.087811     219.66
 H       6.803586     1.046719     0.856730      26.78
 H       5.954616    -0.742132    -0.907954      27.31
 H       6.715234    -0.824352     0.869782      27.25
55
name= lig-ACN-Water-frame_690
 C      -4.513106     1.174658    -2.625190      12.06
 H      -5.021830     0.455617    -3.279232      18.87
 C      -3.823946     2.329547    -0.396688      45.48
 H      -3.857390     2.292984     0.600899      24.61
 C      -3.584065     3.487581    -1.171778      -1.49
 O      -3.171158     4.699974    -0.638174     173.88
 C      -3.097930     4.964329     0.875091      87.85
 H      -2.178226     4.465414     1.458261      24.39
 H      -4.254156     4.824590     1.521076      21.37
 H      -3.089647     6.125079     0.842046      22.25
 C      -3.506677     3.358753    -2.584858       8.41
 O      -3.004936     4.476628    -3.393547     180.85
 H      -2.647253     5.190979    -2.716761      21.27
 C      -4.026314     2.304866    -3.253508      71.93
 H      -3.996778     2.305276    -4.239325      26.36
 C      -4.457794     1.173656    -1.108817      -8.80
 C      -4.645335    -0.155103    -0.358485     100.23
 H      -5.419267    -0.639384    -0.877799      28.52
 O      -5.149578     0.108329     0.891291     224.25
 H      -4.483354     0.252520     1.582976      24.99
 C      -3.417316    -1.139406    -0.559319      76.77
 H      -3.396566    -1.127236    -1.621725      28.60
 C      -3.712347    -2.409431     0.216136     103.55
 O      -4.650602    -3.301779    -0.458152     159.94
 H      -4.077068    -3.323169    -1.439368      26.04
 H      -4.081473    -2.043307     1.060415      28.82
 H      -2.555523    -2.842335     0.428388      24.31
 C       1.116980    -1.046929    -0.994741      51.74
 H       1.702375    -1.633165    -1.667432      22.93
 C       1.279575     0.463706     0.911033      55.47
 H       1.781373     1.299462     1.582860      19.86
 C      -0.102150     0.442585     0.980148       2.64
 O      -0.808591     0.903036     2.088279     178.64
 C      -0.179202     1.146565     3.327826     105.08
 H       0.450299     2.316279     3.511207      21.67
 H      -0.922274     1.507756     4.163497      23.17
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 H       0.636633     0.427431     3.515636      25.36
 C      -0.886271    -0.509018     0.036477       9.32
 O      -2.321022    -0.487084     0.312832     119.02
 C      -0.286681    -1.108193    -0.955158      75.44
 H      -0.656398    -1.818794    -1.751445      24.03
 C       1.891876    -0.179665    -0.209328      36.50
 C       3.388108    -0.082787    -0.452308      94.63
 H       3.528863    -0.409575    -1.399347      27.64
 O       3.660440     1.419191    -0.536385     146.84
 H       4.479912     1.660495    -0.057770      22.16
 C       4.459234    -0.603631     0.608121      80.94
 H       4.263854     0.071181     1.547750      23.79
 O       4.196748    -2.132566     0.945789     261.86
 H       3.892470    -2.582954     0.113077      27.74
 C       5.982223    -0.484011     0.207728      85.34
 O       6.471744     1.010117    -0.089321     171.87
 H       6.857750     1.531012     0.707092      25.86
 H       6.091778    -1.116591    -0.708378      29.88
 H       6.579598    -1.163870     0.938575      29.15
55
name= lig-ACN-Water-frame_691
 C      -4.533751     1.264572    -2.479757      82.44
 H      -4.849067     0.269119    -2.984411      27.07
 C      -4.022583     2.351985    -0.442314      77.29
 H      -3.935759     2.382499     0.638301      19.04
 C      -3.535164     3.496448    -1.128615      14.35
 O      -3.150932     4.692888    -0.561235     216.90
 C      -3.185509     4.927852     0.834477      80.87
 H      -2.239692     4.296775     1.152438      25.06
 H      -4.211295     4.315905     1.391146      21.60
 H      -2.926276     6.038469     1.044499      23.46
 C      -3.579410     3.484715    -2.592890      -1.83
 O      -3.070546     4.414373    -3.337244     182.74
 H      -2.991771     5.216927    -2.772575      25.68
 C      -3.985519     2.281026    -3.343319      43.07
 H      -4.072541     2.346579    -4.399416      15.95
 C      -4.416368     1.230884    -1.154765      23.60
 C      -4.684637    -0.171258    -0.417930      71.05
 H      -5.507784    -0.739233    -0.819645      25.99
 O      -5.154338     0.214253     1.007695     133.81
 H      -4.348791     0.284348     1.644883      22.25
 C      -3.421818    -1.123840    -0.605732      65.34
 H      -3.000222    -1.147025    -1.560320      27.45
 C      -3.621704    -2.487587     0.185735     114.66
 O      -4.596200    -3.340666    -0.448908     184.11
 H      -4.288861    -3.622245    -1.453078      28.89
 H      -3.976225    -2.397272     1.147729      26.93
 H      -2.683996    -3.251270     0.270806      24.71
 C       1.160858    -1.022333    -1.059795      47.65
 H       1.531649    -1.739300    -1.743846      23.11
 C       1.381657     0.399687     0.911125      58.81
 H       2.010080     1.273943     1.121916      21.88
 C      -0.121092     0.429509     0.944259       0.99
 O      -0.916577     0.905708     2.113789     129.66
 C      -0.176352     1.241003     3.411200      88.92
 H       0.381937     2.324126     2.993792      19.97
 H      -1.155913     1.127744     4.033997      23.10
 H       0.416927     0.458856     3.886785      25.92
 C      -0.922079    -0.438333     0.188656       8.48
 O      -2.249442    -0.510797     0.283914     143.71
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 C      -0.258660    -1.107989    -0.988982      39.36
 H      -1.012743    -1.635589    -1.694388      21.80
 C       1.948958    -0.223972    -0.201227      26.68
 C       3.475368    -0.062519    -0.560800      84.72
 H       3.740152    -0.521328    -1.420308      28.93
 O       3.694352     1.451838    -0.565700     141.96
 H       4.272793     1.651448     0.207210      24.33
 C       4.495882    -0.677868     0.589100      73.18
 H       4.272750    -0.219078     1.672256      23.66
 O       4.134450    -2.062337     0.964019     247.49
 H       4.300425    -2.544586     0.063710      28.43
 C       6.004884    -0.504315     0.177159      98.84
 O       6.395922     0.974000    -0.088813     153.53
 H       6.677012     1.067813     0.872584      25.45
 H       6.361908    -1.000193    -0.708699      30.63
 H       6.586578    -0.625100     1.161728      28.61
55
name= lig-ACN-Water-frame_692
 C      -4.513864     1.220189    -2.576447      60.13
 H      -4.822774     0.178112    -3.082599      25.63
 C      -4.146495     2.422565    -0.420510      48.56
 H      -4.096361     2.384032     0.762124      17.21
 C      -3.580238     3.461749    -1.158454      -0.31
 O      -3.147843     4.745035    -0.609369     170.24
 C      -3.158917     4.772811     0.870487      95.81
 H      -2.419836     4.301416     1.566161      24.59
 H      -4.380422     4.454368     1.333815      22.34
 H      -3.302460     5.913529     1.070954      24.43
 C      -3.629515     3.430454    -2.561379      28.10
 O      -3.085305     4.546980    -3.346250     179.34
 H      -2.868450     5.353716    -2.888979      26.16
 C      -4.058697     2.336782    -3.243690      66.86
 H      -3.991058     2.279387    -4.385343      20.70
 C      -4.426004     1.198375    -1.085005     -48.57
 C      -4.662762    -0.037956    -0.392669      74.22
 H      -5.531251    -0.598062    -0.855678      24.04
 O      -5.134580     0.218579     1.023942     143.79
 H      -4.396019     0.195951     1.752780      20.69
 C      -3.312245    -1.082841    -0.403785      91.72
 H      -3.143666    -1.257843    -1.420880      26.98
 C      -3.535057    -2.608971     0.114968     100.05
 O      -4.613957    -3.403907    -0.509355     254.01
 H      -4.128646    -3.746755    -1.226893      32.68
 H      -3.884006    -2.413694     1.145889      25.75
 H      -2.396936    -2.916129     0.061730      23.84
 C       1.201418    -1.083403    -1.169784      37.48
 H       1.678776    -1.321897    -2.092515      23.65
 C       1.289526     0.491275     0.800946      63.77
 H       1.764706     0.833462     1.670699      21.55
 C      -0.101158     0.308045     1.148448      -1.01
 O      -0.903942     0.883807     2.107974     166.31
 C      -0.291845     1.301497     3.350396     111.77
 H       0.395277     2.394758     3.567358      22.10
 H      -0.967914     1.735747     4.214381      23.02
 H       0.446300     0.536895     3.526557      25.98
 C      -0.906567    -0.380168     0.052389      10.92
 O      -2.316125    -0.469771     0.351057     196.74
 C      -0.230685    -1.055872    -0.896267      68.53
 H      -0.778050    -1.774652    -1.592881      22.37
 C       2.054704    -0.384923    -0.254111       2.92
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 C       3.556261     0.006501    -0.477870     102.18
 H       3.761975    -0.244008    -1.447555      26.30
 O       3.744413     1.411280    -0.602943     177.35
 H       3.921347     1.814646     0.318940      23.02
 C       4.451016    -0.705225     0.517003     104.66
 H       4.382591     0.005488     1.461803      24.23
 O       4.121702    -1.999523     0.885517     301.66
 H       4.406780    -2.757225     0.338784      30.48
 C       6.029016    -0.476028     0.222382     108.22
 O       6.297804     0.849752    -0.044787     267.84
 H       6.640035     1.374759     0.648564      29.20
 H       6.195733    -1.091068    -0.652286      31.80
 H       6.710076    -1.050833     0.959342      30.23
55
name= lig-ACN-Water-frame_693
 C      -4.453343     1.127876    -2.534296      38.60
 H      -4.771234     0.332186    -3.365419      20.23
 C      -4.144936     2.436546    -0.418611      56.43
 H      -4.358082     2.426284     0.798831      18.91
 C      -3.672584     3.589637    -1.151767      14.72
 O      -3.134623     4.684630    -0.611938     182.99
 C      -3.259639     4.759312     0.928279      79.22
 H      -2.394708     4.089002     1.143774      25.58
 H      -4.376594     4.166990     1.192809      19.82
 H      -3.036240     5.842000     1.205136      23.96
 C      -3.558898     3.547218    -2.602611     -14.05
 O      -3.129074     4.628088    -3.348339     184.46
 H      -2.788704     5.214557    -2.570442      20.65
 C      -4.160317     2.359507    -3.214831      34.72
 H      -4.040664     2.418182    -4.413251      20.66
 C      -4.479812     1.254183    -1.158355      34.79
 C      -4.596515    -0.115905    -0.201943      93.99
 H      -5.342276    -0.727834    -0.819500      25.80
 O      -5.148783     0.184855     0.993844     235.94
 H      -4.432506     0.204806     1.698339      23.01
 C      -3.374331    -1.072609    -0.346985      85.12
 H      -3.037055    -0.874454    -1.313364      26.27
 C      -3.512657    -2.565573     0.121209     111.61
 O      -4.553248    -3.436828    -0.564494     233.79
 H      -4.189016    -3.584613    -1.395585      32.36
 H      -3.716091    -2.793574     1.253722      25.29
 H      -2.693909    -3.278163    -0.045189      23.46
 C       1.252995    -1.013524    -1.178434      41.62
 H       1.527168    -1.590914    -2.063476      23.63
 C       1.265582     0.391185     0.815999      81.85
 H       1.886007     0.737436     1.514378      19.78
 C      -0.142579     0.185251     1.088149      12.24
 O      -0.870483     0.901748     2.123787     160.49
 C      -0.276115     1.381741     3.349312      95.27
 H       0.328736     2.344901     2.764083      19.82
 H      -1.329619     1.383325     3.926299      21.65
 H       0.266277     0.671274     3.981834      26.01
 C      -0.913380    -0.353550     0.097961       8.03
 O      -2.291702    -0.374093     0.476897     140.68
 C      -0.161080    -1.125637    -0.977913      48.08
 H      -0.787950    -1.702480    -1.690645      20.73
 C       1.981154    -0.288540    -0.224464      24.38
 C       3.512143    -0.045827    -0.534318      78.02
 H       3.759389    -0.516292    -1.448226      24.17
 O       3.764751     1.444901    -0.570047     163.96
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 H       3.895149     1.786902     0.379219      22.50
 C       4.545302    -0.575568     0.575121      99.56
 H       4.240074    -0.173855     1.589443      22.56
 O       4.093068    -2.038120     0.840658     296.30
 H       4.263268    -2.400293    -0.039242      29.16
 C       5.958108    -0.649632     0.196861     106.68
 O       6.296704     0.833885    -0.040811     254.58
 H       6.524683     1.041461     0.888497      30.38
 H       6.172553    -1.087964    -0.747274      31.79
 H       6.501410    -1.074397     1.087951      30.07
55
name= lig-ACN-Water-frame_694
 C      -4.415140     1.243868    -2.521196      -0.36
 H      -4.625518     0.147236    -2.843366      20.81
 C      -4.150511     2.427097    -0.560889      31.35
 H      -4.154074     2.516098     0.674509      18.65
 C      -3.754031     3.585977    -1.199540       8.92
 O      -3.153697     4.729710    -0.498512     222.76
 C      -3.257609     4.712687     0.859334     111.29
 H      -2.665692     3.932921     1.399284      26.48
 H      -4.398081     4.541352     1.456371      21.54
 H      -2.995985     5.702667     1.284727      24.41
 C      -3.639907     3.559836    -2.594694       0.32
 O      -3.170239     4.672870    -3.286513     199.71
 H      -2.659020     5.472700    -2.893079      20.49
 C      -4.110210     2.438794    -3.277782      68.89
 H      -4.343904     2.367022    -4.440361      24.08
 C      -4.470642     1.136257    -1.082076     -11.44
 C      -4.630737    -0.158243    -0.332109      75.59
 H      -5.426095    -0.902541    -0.638457      24.09
 O      -5.214426     0.135195     1.090773     117.52
 H      -4.515167     0.282349     1.776820      23.45
 C      -3.332137    -0.995402    -0.292117      77.38
 H      -3.090856    -1.219827    -1.314871      25.96
 C      -3.501080    -2.628936     0.100255     108.29
 O      -4.495088    -3.374523    -0.599083     206.14
 H      -4.219944    -3.412898    -1.612820      27.30
 H      -3.920565    -2.497136     1.218813      24.48
 H      -2.458887    -2.777148    -0.005493      26.07
 C       1.150170    -0.968406    -1.143518      46.00
 H       1.869511    -1.636098    -1.636506      21.06
 C       1.319852     0.268398     1.000134      79.07
 H       1.728677     1.083394     1.404608      22.39
 C      -0.081195     0.266442     1.033687      -3.31
 O      -0.835661     0.790578     2.069674     129.88
 C      -0.268593     1.451887     3.296484     103.70
 H       0.347044     2.593592     3.396670      21.63
 H      -1.102523     2.088706     3.891086      22.57
 H       0.414038     0.777458     3.854176      25.10
 C      -0.927696    -0.556491     0.103636      13.23
 O      -2.233268    -0.350283     0.524938     147.04
 C      -0.283047    -1.102686    -1.005190      71.91
 H      -0.792685    -1.649298    -1.771197      24.65
 C       1.973696    -0.164959    -0.313173      10.80
 C       3.461639     0.005616    -0.453591      94.33
 H       3.748485    -0.401580    -1.430432      26.67
 O       3.722721     1.459203    -0.570111     174.71
 H       4.147654     1.684742     0.277115      24.39
 C       4.367040    -0.698147     0.643231     104.31
 H       4.508456    -0.108760     1.541751      26.71
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 O       4.099331    -2.052117     0.757804     311.59
 H       3.775968    -2.474431    -0.088718      28.58
 C       5.925505    -0.642289     0.138070     100.59
 O       6.380013     0.752853     0.014800     224.76
 H       6.908235     1.148112     0.816755      26.14
 H       6.028014    -1.321175    -0.693184      32.80
 H       6.599858    -1.043081     0.908845      31.15
55
name= lig-ACN-Water-frame_695
 C      -4.426310     1.268295    -2.552974      93.33
 H      -4.598441     0.559255    -3.367568      25.96
 C      -4.160042     2.397785    -0.457925      66.35
 H      -4.031853     2.401157     0.716829      19.33
 C      -3.717172     3.568159    -1.173878     -22.32
 O      -3.248792     4.700246    -0.541712     170.92
 C      -3.276845     4.717747     1.030533      82.70
 H      -2.798230     3.823982     1.491403      25.23
 H      -4.439303     4.827439     1.087365      23.53
 H      -2.673788     5.607980     1.204826      25.42
 C      -3.739065     3.645337    -2.629488       4.89
 O      -3.207907     4.724150    -3.296360     194.97
 H      -2.847380     5.164540    -2.503532      24.00
 C      -4.081706     2.410353    -3.262798      35.96
 H      -3.976344     2.438785    -4.404783      18.95
 C      -4.407448     1.191383    -1.132985     -25.47
 C      -4.712348    -0.132726    -0.276507      68.87
 H      -5.397512    -0.636766    -1.078047      23.60
 O      -5.274310     0.065666     1.065750     172.28
 H      -4.517449     0.086513     1.665391      25.85
 C      -3.277446    -1.075446    -0.317507      82.43
 H      -2.920183    -0.834223    -1.321501      25.98
 C      -3.468441    -2.486631     0.172568     119.59
 O      -4.432427    -3.267256    -0.647270     220.29
 H      -3.844226    -3.528976    -1.636743      22.47
 H      -3.839207    -2.708887     1.302538      23.42
 H      -2.677557    -3.173692     0.228320      25.71
 C       1.087525    -0.966123    -1.095024      51.93
 H       1.308180    -1.345729    -2.118755      18.16
 C       1.380806     0.427309     0.959285      70.92
 H       1.879260     0.908318     1.794343      20.44
 C      -0.049189     0.241552     1.044983       6.07
 O      -0.796071     0.772759     2.101655     154.20
 C      -0.225980     1.563150     3.217491      95.22
 H       0.609488     2.202871     2.564986      19.94
 H      -1.267517     1.738236     3.872098      21.14
 H       0.181582     0.750156     3.891038      24.40
 C      -0.855068    -0.576179     0.191715      10.17
 O      -2.272972    -0.446232     0.434881     146.83
 C      -0.354931    -1.104338    -1.003872      69.53
 H      -0.877377    -1.755463    -1.652608      24.13
 C       1.892470    -0.148973    -0.204775      30.15
 C       3.414452     0.065138    -0.396421      90.11
 H       3.693150    -0.373754    -1.388476      26.84
 O       3.703741     1.468317    -0.559822     206.22
 H       3.982589     1.943739     0.261555      26.16
 C       4.348042    -0.715426     0.579209      96.78
 H       3.957514    -0.510170     1.533956      26.97
 O       4.035437    -2.167188     0.723028     286.35
 H       3.785749    -2.505437    -0.195091      28.53
 C       5.863895    -0.601818     0.183094     106.17
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 O       6.496908     0.679472     0.012978     235.59
 H       6.939623     0.836571     0.923267      27.28
 H       5.908599    -0.847778    -0.866233      31.02
 H       6.329893    -1.335544     0.804426      30.89
55
name= lig-ACN-Water-frame_696
 C      -4.452073     1.207521    -2.625823      60.60
 H      -4.762871     0.295963    -3.000249      22.93
 C      -4.079911     2.402505    -0.368697      89.49
 H      -4.184367     2.332167     0.711192      19.63
 C      -3.731195     3.515044    -1.111649      -6.87
 O      -3.303491     4.689795    -0.512987     181.50
 C      -3.334927     4.787173     1.021774      89.62
 H      -3.043707     3.735862     1.264922      25.63
 H      -4.180010     5.018419     1.707342      25.31
 H      -2.560030     5.476185     1.363536      27.27
 C      -3.778636     3.648882    -2.542208       2.71
 O      -3.252463     4.768596    -3.255731     194.18
 H      -2.798064     5.492557    -2.824118      22.85
 C      -4.035208     2.455010    -3.294898      42.73
 H      -3.724322     2.375353    -4.309435      21.13
 C      -4.416659     1.238341    -1.162499     -43.85
 C      -4.619504    -0.113758    -0.341391      80.79
 H      -5.499758    -0.866252    -0.693243      21.10
 O      -5.294721    -0.007492     0.943966     125.13
 H      -4.683345     0.224406     1.697110      24.67
 C      -3.336663    -1.071937    -0.426575      59.80
 H      -3.182101    -1.357982    -1.522732      19.86
 C      -3.472152    -2.517983     0.209661     108.85
 O      -4.388552    -3.149624    -0.660180     238.41
 H      -3.805681    -3.475336    -1.653923      21.19
 H      -4.035799    -2.144242     1.186734      22.26
 H      -2.487103    -2.820701     0.323368      25.64
 C       1.046488    -0.922719    -1.149097      27.40
 H       1.657966    -1.043820    -2.061844      21.03
 C       1.247591     0.607314     0.900689      75.35
 H       2.114814     0.778499     1.654192      16.57
 C      -0.080513     0.222308     1.176350      15.96
 O      -0.840783     0.766468     2.158734     203.49
 C      -0.167992     1.505035     3.086657     132.43
 H       0.420539     2.526773     2.795293      23.39
 H      -0.906321     2.435492     3.431458      23.62
 H       0.565966     1.147909     3.876637      25.96
 C      -0.931656    -0.460205     0.231651      15.73
 O      -2.236278    -0.489766     0.465041     122.76
 C      -0.283326    -1.138305    -0.875921      63.74
 H      -0.955673    -1.614054    -1.577599      19.69
 C       1.910702    -0.250081    -0.182286       9.48
 C       3.342319     0.004237    -0.488259      64.84
 H       3.523208    -0.409639    -1.560257      20.92
 O       3.716611     1.516513    -0.523263     171.84
 H       3.667893     1.725441     0.452943      22.32
 C       4.281086    -0.681488     0.614093      90.68
 H       4.333000    -0.240784     1.544544      25.98
 O       3.950062    -2.275359     0.609652     199.20
 H       4.263325    -2.630069    -0.246554      27.89
 C       5.763319    -0.649727     0.131408      99.49
 O       6.622868     0.628893     0.111647     253.48
 H       6.698414     1.125836     0.944786      29.43
 H       5.691803    -1.123746    -0.862391      29.74
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 H       6.385743    -1.272352     0.705352      29.35
55
name= lig-ACN-Water-frame_697
 C      -4.428726     1.271299    -2.552574      59.63
 H      -4.596415     0.451649    -3.120955      26.16
 C      -4.055196     2.306763    -0.423937      56.75
 H      -4.132731     2.314482     0.589712      24.04
 C      -3.756389     3.588085    -1.031997      -2.25
 O      -3.378129     4.793833    -0.377275     241.47
 C      -3.303515     4.781820     0.979189     123.75
 H      -3.056823     3.856933     1.631630      23.48
 H      -4.242159     5.201979     1.152530      23.26
 H      -2.455655     5.499592     1.169281      25.96
 C      -3.660182     3.603138    -2.484762     -25.59
 O      -3.344931     4.750555    -3.205568     199.50
 H      -2.962255     5.362491    -2.547666      23.98
 C      -4.014982     2.391783    -3.287244      46.50
 H      -4.008224     2.539933    -4.298698      18.26
 C      -4.464303     1.162692    -1.132033      38.67
 C      -4.569703    -0.170442    -0.516718      83.66
 H      -5.220506    -0.759800    -1.397662      23.73
 O      -5.256586    -0.035640     0.871850     114.85
 H      -4.560361     0.478825     1.454524      23.77
 C      -3.335389    -1.045502    -0.415035      80.50
 H      -2.796546    -1.024913    -1.471331      23.65
 C      -3.548641    -2.371915     0.205144     118.35
 O      -4.388629    -3.162359    -0.651306     237.99
 H      -4.013748    -3.274117    -1.695071      24.59
 H      -4.057994    -2.574260     1.242187      23.78
 H      -2.677139    -2.903976     0.398171      26.41
 C       1.119160    -0.873491    -1.186808      49.45
 H       1.458946    -1.626758    -1.890657      24.67
 C       1.208887     0.466412     0.847271      69.41
 H       1.533039     1.452035     1.471257      16.83
 C      -0.152241     0.269539     1.192336       8.49
 O      -0.886240     0.747944     2.261065     165.62
 C      -0.072551     1.760555     3.088349      90.30
 H       0.622457     2.109743     2.299831      21.45
 H      -0.918084     2.176393     3.929027      21.69
 H       0.341315     0.944390     3.747753      25.08
 C      -0.889027    -0.445549     0.173576      17.38
 O      -2.296213    -0.468446     0.498284     120.10
 C      -0.287153    -1.108756    -0.800459      69.04
 H      -0.868245    -1.576309    -1.622170      22.28
 C       1.857732    -0.135077    -0.213529      29.91
 C       3.336772     0.007897    -0.464425      83.36
 H       3.711883    -0.351723    -1.537478      23.27
 O       3.669835     1.421492    -0.533266     237.04
 H       4.079306     1.888368     0.270674      23.66
 C       4.251796    -0.781910     0.499713     102.94
 H       3.954017    -0.530159     1.448389      27.77
 O       3.907935    -2.191271     0.524142     292.44
 H       4.293915    -2.579165    -0.295175      29.18
 C       5.825104    -0.680377     0.116166     100.49
 O       6.626471     0.510443     0.162662     263.04
 H       6.685035     0.858564     1.056096      29.67
 H       6.045436    -0.910319    -0.959624      28.43
 H       6.131486    -1.480912     0.735179      30.21
55
name= lig-ACN-Water-frame_698
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 C      -4.395729     1.247264    -2.559647      54.87
 H      -4.695126     0.509537    -3.240529      24.00
 C      -4.066311     2.359328    -0.399414      83.53
 H      -3.951046     2.275235     0.622523      22.99
 C      -3.720622     3.548341    -1.051718       7.96
 O      -3.443533     4.775503    -0.442772     211.72
 C      -3.292308     4.912150     1.124234      90.66
 H      -3.043747     3.798467     1.429903      22.98
 H      -4.098315     5.202549     1.658048      25.67
 H      -2.503751     5.727123     1.354468      25.06
 C      -3.569354     3.568861    -2.454102      12.33
 O      -3.428610     4.700400    -3.122665     215.72
 H      -3.051195     5.524167    -2.631120      21.53
 C      -4.011694     2.461451    -3.156969      64.98
 H      -4.122765     2.467883    -4.195784      22.10
 C      -4.391412     1.193755    -1.216143      34.04
 C      -4.626938    -0.208122    -0.552172      85.23
 H      -5.446152    -1.000501    -1.113903      22.44
 O      -5.204306    -0.089331     0.701710     186.66
 H      -4.519236     0.205852     1.361032      25.77
 C      -3.204079    -0.961336    -0.357362      81.53
 H      -2.747344    -1.114747    -1.472220      24.14
 C      -3.608708    -2.418964     0.178526     114.39
 O      -4.469119    -3.243291    -0.683244     248.30
 H      -3.992048    -3.287815    -1.469332      31.56
 H      -4.107635    -2.029109     1.142227      25.27
 H      -2.677969    -2.855168     0.271795      27.17
 C       1.076048    -0.978282    -1.118274      35.75
 H       1.590726    -1.573754    -1.867191      20.17
 C       1.164034     0.443797     0.906771      51.52
 H       1.977643     1.258843     1.314094      16.47
 C      -0.248715     0.299585     1.112700      22.85
 O      -0.836373     0.814711     2.333355     157.00
 C      -0.044697     1.761798     3.141886     114.43
 H       0.384770     2.535944     2.795788      27.78
 H      -0.880143     2.603565     3.654515      22.64
 H       0.875347     1.426914     3.764249      24.53
 C      -1.012748    -0.445790     0.268614      14.88
 O      -2.332342    -0.377667     0.531024     163.00
 C      -0.291400    -1.068022    -0.973834      58.09
 H      -0.846108    -1.928714    -1.431961      22.68
 C       1.852793    -0.051673    -0.326699       5.41
 C       3.374823     0.030606    -0.493437      89.76
 H       3.345048    -0.507890    -1.563829      24.27
 O       3.676724     1.384912    -0.630353     217.73
 H       3.924485     1.668499     0.302552      24.20
 C       4.278369    -0.805843     0.418728      99.65
 H       4.225595    -0.412845     1.381351      28.11
 O       3.893103    -2.147369     0.409575     322.38
 H       3.727117    -2.579681    -0.497031      28.05
 C       5.856091    -0.802926     0.135410     103.59
 O       6.599400     0.422384     0.230439     245.14
 H       6.899231     0.767240     1.151124      25.81
 H       5.805421    -1.154105    -0.945382      30.52
 H       6.411485    -1.505505     0.703716      31.23
55
name= lig-ACN-Water-frame_699
 C      -4.371775     1.237388    -2.663214      30.05
 H      -4.811519     0.288150    -3.081870      22.87
 C      -4.071054     2.306136    -0.367741      86.52
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 H      -4.203332     2.303233     0.739246      22.94
 C      -3.614871     3.498922    -0.959562     -23.07
 O      -3.500054     4.799894    -0.388564     183.85
 C      -3.291584     4.956088     1.159960     100.70
 H      -2.665240     4.029831     1.529915      24.58
 H      -4.158267     5.093846     1.601277      28.08
 H      -2.499192     5.825791     1.051446      24.03
 C      -3.603172     3.567137    -2.395406     -22.19
 O      -3.457032     4.773496    -3.137770     205.45
 H      -2.920104     5.465772    -2.541896      19.11
 C      -4.010720     2.468308    -3.213821      50.90
 H      -3.878760     2.773082    -4.269096      21.87
 C      -4.323403     1.169846    -1.144185     -11.28
 C      -4.515984    -0.170576    -0.569713      75.23
 H      -5.205226    -0.864435    -1.423808      22.39
 O      -5.249958    -0.141669     0.702199     131.07
 H      -4.624847     0.003905     1.412240      28.28
 C      -3.320362    -1.061194    -0.489676      67.03
 H      -2.680708    -1.049595    -1.534016      22.19
 C      -3.586897    -2.460623     0.130169     118.36
 O      -4.532113    -3.272713    -0.683832     229.98
 H      -4.219976    -3.545054    -1.488130      30.99
 H      -4.271551    -2.448108     1.022207      25.46
 H      -2.810887    -3.022124     0.596809      27.19
 C       1.033181    -1.042025    -1.070842      30.88
 H       1.552454    -1.386125    -1.971969      16.82
 C       1.200133     0.534273     0.833956      77.83
 H       1.624363     0.634993     1.918356      18.49
 C      -0.108404     0.395954     1.158566      -2.43
 O      -0.722686     0.893051     2.339236     174.47
 C      -0.049503     1.833805     3.194828     105.93
 H       0.283743     2.378176     2.502598      26.75
 H      -0.961319     2.023040     4.108299      21.52
 H       0.686273     1.246516     3.881174      23.94
 C      -1.007321    -0.448372     0.185629      -1.19
 O      -2.383462    -0.290394     0.554143     110.84
 C      -0.474091    -1.076354    -0.914544      76.66
 H      -0.943081    -1.876254    -1.533059      23.42
 C       1.784090    -0.136880    -0.245948      30.46
 C       3.299529    -0.022502    -0.658454      62.30
 H       3.762560    -0.339672    -1.709545      21.61
 O       3.779547     1.458291    -0.747160     185.44
 H       3.786266     1.919612     0.121030      26.03
 C       4.377305    -0.749408     0.450326      83.56
 H       4.187969    -0.402182     1.433488      25.68
 O       3.826693    -2.226607     0.330657     256.64
 H       3.825088    -2.279816    -0.678210      25.65
 C       5.853217    -0.932751     0.097709     104.58
 O       6.593144     0.391987     0.236334     264.44
 H       6.596538     0.628063     1.223545      29.36
 H       6.203294    -1.269478    -0.931140      28.90
 H       6.090773    -1.719585     0.829689      29.17
55
name= lig-ACN-Water-frame_700
 C      -4.326604     1.288602    -2.572135      69.61
 H      -4.463234     0.484448    -3.423966      21.99
 C      -4.013325     2.289401    -0.319152      56.15
 H      -4.363693     2.059249     0.777306      22.55
 C      -3.595769     3.533010    -0.910601     -14.87
 O      -3.540558     4.762067    -0.251100     231.56
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 C      -3.220595     4.962840     1.052177     130.99
 H      -2.664699     4.242049     1.705071      26.55
 H      -4.125498     4.982439     1.496085      26.87
 H      -3.007868     6.091238     1.267038      24.65
 C      -3.668173     3.614972    -2.424656     -22.39
 O      -3.455011     4.793241    -3.108554     174.53
 H      -2.897095     5.505787    -2.555657      22.61
 C      -3.954670     2.484384    -3.281091      39.46
 H      -4.030509     2.489007    -4.457917      18.54
 C      -4.262761     1.182471    -1.229718      18.08
 C      -4.537586    -0.222075    -0.589401      53.30
 H      -5.393604    -0.676400    -1.416320      22.56
 O      -5.328381    -0.198363     0.761162     113.83
 H      -4.594257     0.041575     1.423288      26.84
 C      -3.318977    -1.135439    -0.453415      72.67
 H      -2.895172    -1.219697    -1.591028      24.25
 C      -3.656253    -2.546146     0.106393     124.55
 O      -4.576777    -3.304643    -0.696183     221.00
 H      -4.052635    -3.398474    -1.634983      26.28
 H      -4.062139    -2.242252     1.061210      27.17
 H      -2.635928    -2.959208    -0.005623      25.04
 C       0.864672    -0.976841    -1.064731      46.09
 H       1.118178    -1.673318    -1.908649      24.01
 C       1.327203     0.531271     0.891286      41.07
 H       2.192540     0.999003     1.476849      19.58
 C      -0.148811     0.394655     1.113134      24.78
 O      -0.706122     0.867931     2.285190     168.91
 C      -0.029678     1.801119     3.241215     110.91
 H       0.398253     2.720421     3.165151      26.60
 H      -0.924759     2.389475     3.976772      23.18
 H       0.874524     1.306987     3.703336      25.61
 C      -1.028853    -0.248402     0.266831      18.62
 O      -2.391241    -0.337199     0.429162     158.57
 C      -0.455877    -1.144055    -0.774018      62.58
 H      -1.173388    -1.400971    -1.530382      22.15
 C       1.859731    -0.254351    -0.249827       1.46
 C       3.412797     0.066295    -0.620032      84.44
 H       3.289372    -0.497961    -1.652284      23.87
 O       3.818472     1.473872    -0.867439     195.25
 H       4.118899     1.780141     0.037988      26.60
 C       4.243662    -0.863400     0.261901      98.44
 H       4.116291    -0.573510     1.313618      26.81
 O       3.794497    -2.198088     0.302087     287.74
 H       4.019517    -2.792725    -0.423264      29.76
 C       5.880173    -0.896081     0.120209      98.42
 O       6.579183     0.284835     0.223206     300.48
 H       6.571972     0.749547     1.034899      30.04
 H       6.038507    -1.355738    -0.912688      28.58
 H       6.301859    -1.556653     0.950480      28.36
55
name= lig-ACN-Water-frame_703
 C      -4.177227     1.246761    -2.550960      59.53
 H      -4.311967     0.256955    -3.055606      21.24
 C      -3.952414     2.238226    -0.339544      59.31
 H      -3.986996     2.159265     0.837725      20.95
 C      -3.730715     3.576299    -0.934862     -36.23
 O      -3.505715     4.861616    -0.255825     222.40
 C      -3.297097     4.803128     1.075809     144.13
 H      -2.260345     4.554251     1.226615      27.80
 H      -3.822498     3.886560     1.555387      24.02
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 H      -3.396165     5.761648     1.560486      26.82
 C      -3.694291     3.667138    -2.407402     -15.25
 O      -3.394539     4.927798    -3.059530     176.93
 H      -3.059689     5.585904    -2.424336      23.31
 C      -3.812078     2.437113    -3.111244      60.70
 H      -3.778013     2.150331    -4.239045      21.51
 C      -4.267185     1.143507    -1.137697      16.14
 C      -4.636546    -0.256885    -0.515182      76.27
 H      -5.412701    -1.049098    -0.996811      21.97
 O      -5.412483    -0.206487     0.804495     113.42
 H      -4.978531     0.176647     1.590212      26.58
 C      -3.349517    -1.142727    -0.453633      70.78
 H      -2.897233    -1.219667    -1.439340      23.70
 C      -3.581681    -2.581271    -0.044156     122.87
 O      -4.571281    -3.270640    -0.813043     238.17
 H      -4.274444    -3.314910    -1.692144      30.57
 H      -3.662509    -2.764472     1.029579      26.50
 H      -2.614185    -3.259339    -0.178546      24.33
 C       1.030812    -0.975249    -1.146957      27.11
 H       1.629724    -1.618191    -1.833082      19.37
 C       1.249609     0.606987     0.803510      73.94
 H       1.777302     0.634118     1.642563      18.84
 C      -0.143204     0.383613     1.138644     -15.92
 O      -0.841681     1.085447     2.274805     136.70
 C       0.147511     1.680288     3.310550      95.66
 H       0.493950     2.641278     2.849743      24.48
 H      -0.726234     1.449280     4.170128      22.52
 H       0.715706     0.883829     3.700986      27.49
 C      -1.006449    -0.445851     0.224976       7.20
 O      -2.391277    -0.345611     0.598302      72.61
 C      -0.339461    -1.126687    -0.831985      68.20
 H      -0.928347    -1.541200    -1.641622      21.32
 C       1.830585    -0.040768    -0.322398      13.97
 C       3.361476    -0.097142    -0.674003     103.78
 H       3.510686    -0.423889    -1.723695      24.37
 O       3.840754     1.196330    -0.799153     249.05
 H       3.983441     1.718275     0.003189      28.14
 C       4.167599    -0.996805     0.204912      97.29
 H       3.877280    -0.461602     1.235474      23.89
 O       3.721250    -2.269367     0.285439     298.92
 H       4.059147    -2.678284    -0.613255      26.30
 C       5.792382    -0.916292     0.084127      95.54
 O       6.583807     0.224237     0.031689     264.25
 H       6.541232     0.613404     0.902461      32.42
 H       6.029048    -1.392446    -0.892818      29.99
 H       6.294162    -1.773616     0.848777      27.99
55
name= lig-ACN-Water-frame_704
 C      -4.220721     1.204930    -2.495948      63.40
 H      -4.286588     0.380080    -3.156710      23.74
 C      -4.028477     2.393278    -0.295939      74.06
 H      -4.187477     2.316786     0.790920      22.15
 C      -3.643156     3.573804    -0.956172      15.79
 O      -3.525659     4.838266    -0.377093     165.93
 C      -3.268858     4.658238     1.188155     104.73
 H      -2.201264     4.609937     1.234227      26.53
 H      -3.842814     3.712523     1.793315      20.94
 H      -3.723146     5.533763     1.593808      25.97
 C      -3.650133     3.620664    -2.371115       1.41
 O      -3.414265     4.835359    -3.028056     205.93
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 H      -3.007537     5.503465    -2.425819      23.61
 C      -3.745705     2.448591    -3.169446      42.24
 H      -3.547281     2.827356    -4.195876      20.54
 C      -4.265796     1.157330    -1.069936      -5.93
 C      -4.606751    -0.218253    -0.423678      88.51
 H      -5.198999    -0.699030    -1.316505      23.92
 O      -5.423883    -0.182597     0.778971     180.86
 H      -4.675457    -0.050130     1.484836      25.76
 C      -3.245095    -0.988925    -0.322711      88.94
 H      -2.848698    -0.848078    -1.268684      26.42
 C      -3.505146    -2.597203    -0.015027     109.25
 O      -4.562965    -3.266244    -0.872825     202.96
 H      -4.325200    -3.301546    -1.727856      33.01
 H      -3.985859    -2.707561     0.966065      25.40
 H      -2.415701    -2.966351    -0.279478      23.80
 C       0.956499    -0.865354    -1.119336      58.52
 H       1.369750    -1.357572    -1.991720      24.01
 C       1.225507     0.547277     0.806513      79.29
 H       1.708537     1.409628     1.088470      19.63
 C      -0.186417     0.433925     1.056942      -0.57
 O      -0.799585     1.055573     2.175227     200.83
 C       0.095023     1.510237     3.281535      91.57
 H       0.661136     2.562504     3.019418      22.75
 H      -0.449220     2.127443     4.294047      22.18
 H       0.989004     1.004773     3.367284      27.12
 C      -0.954816    -0.444422     0.249090      14.51
 O      -2.307631    -0.520652     0.555948     196.17
 C      -0.437279    -1.190522    -0.866431      75.38
 H      -1.068085    -1.638965    -1.692703      20.62
 C       1.765790    -0.169290    -0.294336      35.26
 C       3.256573    -0.079748    -0.587612      80.38
 H       3.263746    -0.568501    -1.546225      22.83
 O       3.916348     1.311696    -0.792389     212.39
 H       4.135337     1.639442     0.119153      26.22
 C       4.257361    -0.955664     0.354730      74.31
 H       4.187990    -0.790138     1.548182      23.72
 O       3.739535    -2.380289     0.278341     260.38
 H       4.007386    -2.884424    -0.558791      27.44
 C       5.732986    -1.023735    -0.003935      88.25
 O       6.529972     0.246612     0.014112     230.36
 H       6.453198     0.872480     0.747715      29.80
 H       5.869519    -1.421817    -1.025336      28.88
 H       6.102530    -1.788132     0.923595      26.69
55
name= lig-ACN-Water-frame_705
 C      -4.121738     1.290524    -2.497765      33.67
 H      -4.501637     0.498088    -2.998382      24.37
 C      -4.117167     2.418267    -0.324739     103.06
 H      -4.250056     2.388656     0.672597      22.41
 C      -3.657533     3.552740    -0.990546      13.33
 O      -3.530126     4.738703    -0.309649     210.03
 C      -3.227537     4.666986     1.194778     116.16
 H      -2.159423     4.650722     1.567128      25.44
 H      -3.828861     3.585488     1.391945      19.89
 H      -3.736295     5.518007     1.562922      24.99
 C      -3.499185     3.574429    -2.359080       8.45
 O      -3.424445     4.751294    -3.017775     200.09
 H      -2.948124     5.456163    -2.437096      22.02
 C      -3.777856     2.458348    -3.143043      58.37
 H      -3.654784     2.346646    -4.181850      21.86
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 C      -4.317118     1.256491    -1.028039      -0.36
 C      -4.528609    -0.091818    -0.378410      97.83
 H      -5.158821    -0.725356    -1.107914      23.90
 O      -5.382250    -0.163407     0.769145     198.29
 H      -4.946217    -0.185492     1.678909      23.54
 C      -3.292577    -1.034825    -0.360640      72.57
 H      -2.916345    -0.937527    -1.293723      26.17
 C      -3.480651    -2.563425    -0.062365     112.88
 O      -4.499844    -3.219958    -0.895295     232.04
 H      -4.057190    -3.093873    -1.844352      25.99
 H      -3.693854    -2.578623     1.047207      25.71
 H      -2.525713    -3.243703     0.053447      24.65
 C       0.865298    -0.948022    -1.187462      64.71
 H       1.198809    -1.189434    -2.153853      21.27
 C       1.157228     0.592270     0.813862      71.48
 H       1.619259     1.543684     1.003937      18.16
 C      -0.173434     0.430557     1.041915      15.68
 O      -0.758404     1.014578     2.127621     201.85
 C       0.113040     1.462654     3.117761      67.05
 H       0.565115     2.515506     2.703453      21.42
 H      -0.759947     1.534617     4.206235      21.68
 H       0.692824     0.630560     3.457355      24.98
 C      -0.971996    -0.460117     0.264695      20.86
 O      -2.238993    -0.637180     0.668501     173.66
 C      -0.448351    -1.054141    -0.871223      64.26
 H      -1.045613    -1.974821    -1.246307      22.18
 C       1.792178    -0.194720    -0.230073      45.75
 C       3.322786    -0.080600    -0.558055      80.28
 H       3.552694    -0.517816    -1.484677      26.03
 O       3.884934     1.364483    -0.748224     189.22
 H       4.120657     1.785553     0.172708      24.60
 C       4.211760    -0.945480     0.454489      72.82
 H       4.163133    -0.549154     1.601238      24.18
 O       3.779246    -2.495844     0.300798     208.30
 H       3.684949    -2.419148    -0.649417      28.94
 C       5.716591    -1.052709    -0.050390      93.57
 O       6.453281     0.242850    -0.009021     154.53
 H       6.334138     0.497360     0.992496      29.50
 H       5.758937    -1.472363    -1.079320      31.81
 H       6.459880    -1.836351     0.601660      29.07
55
name= lig-ACN-Water-frame_706
 C      -4.135482     1.232249    -2.402052      73.24
 H      -4.246607     0.407158    -2.984384      26.71
 C      -4.178080     2.368708    -0.292694     103.67
 H      -4.392687     2.345758     0.680897      24.55
 C      -3.701818     3.539527    -0.906100     -27.35
 O      -3.453476     4.733418    -0.196549     205.09
 C      -3.266173     4.690383     1.157070     125.39
 H      -2.094679     4.693308     1.101760      24.82
 H      -3.616638     3.887924     1.989607      22.61
 H      -3.667243     5.644324     1.552989      25.24
 C      -3.414012     3.562495    -2.414399     -34.05
 O      -3.350116     4.806966    -3.069915     177.76
 H      -2.936157     5.507620    -2.497115      19.52
 C      -3.772070     2.400666    -3.166410      52.75
 H      -3.821593     2.456213    -4.157325      24.75
 C      -4.322171     1.253875    -1.076121      72.92
 C      -4.533116    -0.130900    -0.398461      83.69
 H      -5.200819    -0.667425    -1.159945      25.87
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 O      -5.366806    -0.126524     0.841189     193.71
 H      -4.712800    -0.003420     1.562568      26.23
 C      -3.237617    -1.098632    -0.421007      63.86
 H      -2.742233    -1.012869    -1.295402      26.98
 C      -3.526875    -2.534660    -0.019686     111.50
 O      -4.405097    -3.144558    -0.894350     189.10
 H      -4.182238    -3.199137    -2.023240      23.81
 H      -4.078521    -2.752933     0.945569      24.66
 H      -2.434427    -2.919874    -0.243282      23.59
 C       1.030192    -0.927645    -1.164357      22.74
 H       1.470449    -1.593800    -1.846768      20.41
 C       1.239323     0.640474     0.664410      78.60
 H       1.807362     0.864040     1.615708      17.92
 C      -0.167182     0.376878     1.044423      16.81
 O      -0.850146     0.977366     2.059813     186.18
 C       0.097692     1.397460     3.083504      83.25
 H       0.764374     2.467834     3.086304      23.11
 H      -0.800283     1.753446     4.139521      22.05
 H       0.894851     0.725651     3.328375      27.06
 C      -1.013974    -0.454444     0.281195       4.66
 O      -2.310590    -0.714943     0.808762     187.22
 C      -0.454667    -1.027654    -0.858167      62.61
 H      -1.055894    -1.785347    -1.529143      21.03
 C       1.808124    -0.166700    -0.361146      55.98
 C       3.406672    -0.067481    -0.532769      86.11
 H       3.545462    -0.413512    -1.516358      27.13
 O       3.761710     1.327529    -0.652906     243.84
 H       4.044979     1.754208     0.258520      25.24
 C       4.216126    -1.079406     0.398489      95.12
 H       3.888140    -0.794947     1.516863      24.48
 O       3.821701    -2.415544     0.338310     301.73
 H       3.564586    -2.740445    -0.541223      29.20
 C       5.701355    -1.013168    -0.048231      98.34
 O       6.355597     0.198017     0.012486     190.53
 H       6.695725     0.555180     0.876058      29.75
 H       5.594602    -1.160192    -1.160981      32.31
 H       6.182796    -1.994941     0.535944      29.11
55
name= lig-ACN-Water-frame_707
 C      -4.145348     1.141967    -2.524462      42.28
 H      -4.116737     0.199657    -3.027286      22.72
 C      -4.193914     2.400004    -0.229057      79.01
 H      -4.454419     2.410903     0.800653      23.43
 C      -3.682661     3.543646    -0.909852       9.17
 O      -3.468396     4.714794    -0.272992     176.35
 C      -3.148842     4.800323     1.290248     101.88
 H      -1.992661     4.714249     1.682430      24.60
 H      -3.756694     3.969393     1.640109      24.68
 H      -3.596388     5.841252     1.532227      24.18
 C      -3.516316     3.621840    -2.364944       5.26
 O      -3.224388     4.830488    -3.106673     188.83
 H      -2.843110     5.471139    -2.493469      24.10
 C      -3.728570     2.437442    -3.126198      47.17
 H      -3.653045     2.541060    -4.120237      23.57
 C      -4.304918     1.082888    -0.984895     -69.10
 C      -4.618210    -0.263895    -0.443541      97.60
 H      -5.294999    -0.793905    -1.123611      23.61
 O      -5.309337    -0.083215     0.836630     214.29
 H      -4.796275    -0.163767     1.667564      23.10
 C      -3.282793    -1.032579    -0.233388      95.80
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 H      -2.805386    -0.884382    -1.154305      25.48
 C      -3.491652    -2.539321    -0.023748     111.61
 O      -4.449563    -3.163692    -0.975458     171.94
 H      -3.856857    -2.990672    -1.958354      21.67
 H      -3.855832    -2.462565     1.085669      24.40
 H      -2.535586    -3.182769     0.243997      24.13
 C       1.023488    -0.962395    -1.121529      37.74
 H       1.398545    -1.673538    -1.840468      18.42
 C       1.233327     0.535308     0.680636      88.12
 H       2.111115     0.898662     1.417845      13.42
 C      -0.144087     0.379649     0.962917      23.45
 O      -0.851902     0.982384     2.071522     194.46
 C       0.022349     1.413353     3.179564      48.23
 H       0.397805     2.359559     2.471535      18.78
 H      -0.493701     1.677297     4.482385      20.96
 H       0.728691     0.574431     3.369117      23.74
 C      -0.999602    -0.476764     0.239092      12.00
 O      -2.358462    -0.726387     0.758515     193.23
 C      -0.310307    -1.089352    -0.901263      72.33
 H      -0.883716    -1.550623    -1.780142      20.22
 C       1.909366    -0.071594    -0.430976      45.25
 C       3.319764    -0.134565    -0.622593      92.06
 H       3.579322    -0.517631    -1.601018      24.00
 O       3.686653     1.304474    -0.525821     212.37
 H       4.017605     1.532226     0.421341      22.80
 C       4.204829    -1.015849     0.361797      85.84
 H       4.358373    -0.698198     1.478585      23.75
 O       3.778875    -2.429353     0.347813     260.97
 H       4.093570    -2.687356    -0.615044      25.75
 C       5.627917    -1.062126    -0.070195     103.63
 O       6.356809     0.266305     0.056673     205.34
 H       6.443979     0.435254     0.987165      34.08
 H       5.791911    -1.416950    -1.157724      31.44
 H       6.337408    -1.835511     0.521511      30.17
55
name= lig-ACN-Water-frame_708
 C      -4.063064     1.233354    -2.440098      84.13
 H      -4.292999     0.431515    -3.197932      23.86
 C      -4.162718     2.248826    -0.350656      77.73
 H      -4.299847     2.268881     0.782213      24.68
 C      -3.695801     3.509471    -0.901121     -44.19
 O      -3.417180     4.805334    -0.227673     178.74
 C      -3.161619     4.861774     1.238808     107.04
 H      -1.976334     4.489248     1.325201      23.56
 H      -3.736656     4.282451     1.901762      26.52
 H      -3.380553     6.016125     1.621402      24.34
 C      -3.631277     3.647601    -2.362962      -5.61
 O      -3.104139     4.757742    -3.045564     128.10
 H      -2.960910     5.547657    -2.448119      21.08
 C      -3.742610     2.409055    -3.044721      53.35
 H      -3.384245     2.364417    -4.036266      22.75
 C      -4.296307     1.136711    -1.138680      41.63
 C      -4.639472    -0.304936    -0.331726     102.27
 H      -5.156920    -1.007436    -0.920226      27.41
 O      -5.397030    -0.071636     0.813546     175.22
 H      -4.749676    -0.113938     1.546407      25.53
 C      -3.306118    -1.119997    -0.278575      71.08
 H      -2.984710    -1.009319    -1.341633      25.96
 C      -3.554400    -2.595207     0.043316     113.12
 O      -4.424492    -3.176952    -0.976560     129.94
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 H      -4.127691    -3.115353    -2.015088      24.70
 H      -4.270313    -2.931060     0.882494      24.19
 H      -2.554164    -3.130555    -0.087108      25.41
 C       1.043418    -1.048306    -1.210182      45.49
 H       1.533752    -1.251520    -2.198640      17.67
 C       1.253681     0.454035     0.795214      89.29
 H       1.482672     1.577713     1.179225      15.47
 C      -0.164486     0.401165     1.015666      -4.48
 O      -0.834706     0.935494     2.112908     164.00
 C       0.017701     1.450986     3.147410      71.03
 H       0.688769     2.467700     3.312481      21.59
 H      -1.144843     1.630680     3.987087      21.35
 H       0.790997     0.695582     3.565812      24.64
 C      -0.937577    -0.500981     0.154868      16.44
 O      -2.235473    -0.592881     0.669110     132.58
 C      -0.379747    -1.153727    -0.908872      77.03
 H      -0.951955    -1.928289    -1.442674      24.39
 C       1.760945    -0.177361    -0.368436      17.47
 C       3.350435    -0.108060    -0.641945      83.18
 H       3.570137    -0.293474    -1.724464      24.23
 O       3.675257     1.281579    -0.492922     234.71
 H       4.062079     1.612874     0.356706      25.96
 C       4.188790    -0.967645     0.326435      70.21
 H       3.850797    -0.474943     1.299042      24.32
 O       3.721245    -2.444736     0.320649     259.03
 H       4.018136    -2.828603    -0.566354      29.41
 C       5.770179    -1.007602    -0.101993      91.47
 O       6.328277     0.273029     0.070337     243.16
 H       6.306734     0.623496     1.036315      30.54
 H       5.914355    -1.360055    -1.192464      29.89
 H       6.098742    -1.774036     0.736224      28.75
55
name= lig-ACN-Water-frame_709
 C      -4.042123     1.197519    -2.509115      10.12
 H      -4.153591     0.235360    -3.215186      21.56
 C      -4.039088     2.319970    -0.354886      27.08
 H      -4.053363     2.020103     0.801388      20.24
 C      -3.769735     3.593816    -0.863949      20.87
 O      -3.444270     4.787107    -0.210483     254.16
 C      -3.154270     4.866504     1.139576     107.12
 H      -1.986875     4.426592     1.400984      23.46
 H      -3.840142     4.395685     1.715555      25.78
 H      -2.976292     6.091069     1.281622      23.17
 C      -3.603878     3.636271    -2.291852     -14.05
 O      -3.016030     4.677066    -2.942248      63.46
 H      -3.113766     5.506756    -2.337651      19.65
 C      -3.698712     2.494128    -3.099580      52.22
 H      -3.489030     2.584679    -4.219603      20.63
 C      -4.370694     1.039180    -1.081159      -7.18
 C      -4.571636    -0.217403    -0.433252      89.72
 H      -5.242404    -0.615350    -1.059855      25.31
 O      -5.514172    -0.073559     0.873770      70.70
 H      -5.015375     0.244086     1.684105      26.74
 C      -3.309677    -1.169065    -0.302668      67.73
 H      -2.871246    -1.346406    -1.347070      23.68
 C      -3.610910    -2.720460     0.026452     129.58
 O      -4.432019    -3.255367    -0.992549     189.44
 H      -4.007994    -3.021220    -1.817071      28.83
 H      -3.880946    -2.782271     1.168405      25.02
 H      -2.588591    -3.160651     0.207255      25.11
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 C       0.943182    -1.041726    -1.268083      47.77
 H       1.367866    -1.617199    -2.199140      22.86
 C       1.177889     0.504074     0.791381      61.94
 H       2.041213     1.214656     1.263750      16.25
 C      -0.141042     0.293724     1.059139      25.66
 O      -0.771866     0.921649     2.078542     197.68
 C      -0.093883     1.461548     3.249362      57.71
 H       0.281072     2.526706     2.743207      20.70
 H      -1.000264     1.738081     4.337777      21.53
 H       0.708337     0.657277     3.660781      23.46
 C      -0.884153    -0.474944     0.185327      11.41
 O      -2.238275    -0.486066     0.512936     132.77
 C      -0.413735    -1.289969    -0.952296      53.26
 H      -1.044429    -2.021391    -1.353470      22.63
 C       1.801276    -0.330461    -0.273365      24.04
 C       3.252865    -0.031103    -0.633895      82.74
 H       3.352226    -0.421277    -1.703018      21.60
 O       3.696748     1.349870    -0.536320     260.62
 H       3.964765     1.478306     0.385927      24.74
 C       4.168551    -1.070455     0.189563     105.42
 H       4.151342    -0.841796     1.280840      24.76
 O       3.704298    -2.367231     0.282768     318.19
 H       3.531635    -2.678901    -0.602978      30.13
 C       5.718751    -0.968605     0.047268     101.68
 O       6.359633     0.321462     0.041382     241.34
 H       6.670122     0.667813     0.983856      27.81
 H       5.893876    -1.250852    -1.060455      30.06
 H       6.395072    -1.759325     0.566763      29.87
55
name= lig-ACN-Water-frame_710
 C      -4.095310     1.206870    -2.564956      75.00
 H      -4.012230     0.162728    -3.159285      23.00
 C      -3.999092     2.323869    -0.227878      35.54
 H      -3.877752     2.469668     0.955481      19.49
 C      -3.815672     3.545792    -0.864176      -2.28
 O      -3.525126     4.768327    -0.314206     171.01
 C      -3.078795     4.854402     1.136778     101.79
 H      -2.263047     4.016685     1.481248      24.69
 H      -3.921590     4.732231     1.699516      26.50
 H      -2.941739     6.079598     1.391457      23.47
 C      -3.479064     3.562355    -2.280880     -19.32
 O      -2.955378     4.707254    -2.852055     136.03
 H      -2.801207     5.551377    -2.314149      19.90
 C      -3.721937     2.419008    -3.084268      50.97
 H      -3.593525     2.709771    -4.241770      22.76
 C      -4.205339     1.264427    -1.140199      20.17
 C      -4.662453    -0.242921    -0.428949      59.96
 H      -5.200252    -0.831870    -0.998943      30.47
 O      -5.493786    -0.058251     0.802833     118.76
 H      -4.773493     0.061738     1.535176      26.09
 C      -3.288810    -1.192900    -0.328595      88.20
 H      -3.039896    -1.063900    -1.468641      29.96
 C      -3.510518    -2.681135     0.127951     111.50
 O      -4.436189    -3.372443    -0.980636     159.90
 H      -4.193325    -3.165726    -1.795591      36.35
 H      -4.363492    -2.744011     0.917101      27.05
 H      -2.739072    -3.382995     0.044153      28.65
 C       0.936352    -1.060620    -1.153966      49.57
 H       1.474984    -1.756803    -1.928388      23.22
 C       1.312085     0.410223     0.685639      70.64
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 H       1.882734     0.617730     1.649780      20.04
 C      -0.068437     0.228443     1.079570      -9.06
 O      -0.864001     0.892387     2.125159     153.58
 C      -0.157615     1.502802     3.241764      73.02
 H       0.405713     2.555364     3.079944      23.26
 H      -1.187067     1.694635     4.257783      22.23
 H       0.809553     0.872961     3.686702      24.47
 C      -0.993810    -0.588610     0.147171      11.96
 O      -2.384308    -0.438016     0.384405     155.37
 C      -0.399612    -1.275154    -0.864475      79.01
 H      -0.908860    -1.718143    -1.631273      26.71
 C       1.755747    -0.336949    -0.359271      41.90
 C       3.231021    -0.119393    -0.639280      75.36
 H       3.403877    -0.142130    -1.790845      22.67
 O       3.680741     1.382964    -0.589504     170.11
 H       4.108574     1.712841     0.248019      25.89
 C       4.197564    -0.966396     0.319270      94.60
 H       3.922976    -0.533584     1.266365      26.69
 O       3.667052    -2.382040     0.174394     285.77
 H       3.675694    -2.530651    -0.815066      27.45
 C       5.718173    -1.002724    -0.034966      97.27
 O       6.413943     0.401993     0.041731     182.28
 H       6.569130     0.579182     0.982483      30.57
 H       5.981378    -1.496389    -1.012079      30.65
 H       6.048380    -1.621182     0.889883      29.13
55
name= lig-ACN-Water-frame_711
 C      -4.101849     1.281683    -2.422506      26.86
 H      -4.526271     0.396170    -3.111324      23.49
 C      -4.018469     2.317337    -0.201555      31.94
 H      -4.290461     1.998790     0.878194      21.23
 C      -3.686347     3.532502    -0.926202      16.15
 O      -3.557903     4.838643    -0.290360     155.88
 C      -3.166165     4.828608     1.090145     109.43
 H      -2.363133     3.966517     1.145951      25.79
 H      -3.899964     4.710131     1.862152      26.67
 H      -2.309016     5.698614     1.131149      24.05
 C      -3.404283     3.538692    -2.311224      10.94
 O      -2.903215     4.712609    -2.845964     203.12
 H      -2.941515     5.261903    -2.071153      23.35
 C      -3.715367     2.471801    -3.158296      49.70
 H      -3.458476     2.305020    -4.343146      21.54
 C      -4.127241     1.135046    -1.042990      -4.37
 C      -4.656830    -0.260338    -0.486974     111.77
 H      -5.354243    -0.481834    -1.159806      29.46
 O      -5.320624    -0.027464     0.709313     136.42
 H      -4.777208    -0.085491     1.519252      25.33
 C      -3.438190    -1.158349    -0.450689      81.47
 H      -3.013862    -1.397816    -1.558006      25.31
 C      -3.575034    -2.656003     0.031306     129.11
 O      -4.401616    -3.435905    -0.897483     187.32
 H      -3.947906    -3.275954    -1.807531      27.81
 H      -4.027441    -2.722251     1.110276      26.57
 H      -2.637867    -2.827757     0.436492      27.51
 C       1.032101    -1.207415    -1.106488      47.80
 H       1.351105    -1.634655    -2.147968      18.81
 C       1.218940     0.244138     0.873035      67.79
 H       1.895974     0.965105     1.339287      18.59
 C      -0.215428     0.200608     1.049992      14.01
 O      -0.870213     0.815782     2.120517     176.25
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 C      -0.165449     1.535052     3.210413      69.15
 H       0.119996     2.596754     3.008678      23.41
 H      -1.293552     1.519266     4.103390      22.24
 H       0.578494     0.691440     3.717755      22.94
 C      -1.041851    -0.546764     0.256227      22.29
 O      -2.420917    -0.383949     0.387390     129.88
 C      -0.452623    -1.236807    -0.878365      57.45
 H      -1.074820    -1.763207    -1.552092      24.10
 C       1.855692    -0.219978    -0.435062       5.90
 C       3.381992    -0.064130    -0.702242      78.33
 H       3.713758    -0.733050    -1.628911      21.65
 O       3.614883     1.356841    -0.643447     235.62
 H       3.930415     1.455118     0.326108      22.80
 C       4.121779    -0.882008     0.292111      96.86
 H       4.016736    -0.778309     1.305437      28.83
 O       3.694794    -2.329625     0.099160     267.62
 H       4.070543    -2.715704    -0.797427      29.44
 C       5.750460    -0.901834     0.021975      98.22
 O       6.406998     0.336290     0.017638     292.81
 H       6.438409     0.740534     0.880342      33.21
 H       5.952444    -1.373318    -0.956980      32.56
 H       6.245122    -1.601730     0.776427      30.42
55
name= lig-ACN-Water-frame_712
 C      -4.106840     1.321947    -2.408762      51.29
 H      -4.607727     0.477723    -3.006022      27.60
 C      -4.024012     2.279887    -0.291438      68.46
 H      -4.352762     2.535929     0.718284      26.68
 C      -3.569413     3.517586    -0.883537     -51.34
 O      -3.637499     4.830157    -0.310902     200.75
 C      -3.079034     4.750304     1.050635     108.45
 H      -2.750117     3.737948     1.327918      25.38
 H      -4.018338     5.016931     1.602770      24.29
 H      -2.452615     5.722287     1.313461      24.57
 C      -3.354380     3.579419    -2.341917      -1.66
 O      -2.857022     4.701119    -2.882178     104.96
 H      -2.808066     5.610409    -2.471855      24.52
 C      -3.679489     2.422475    -3.098712      65.67
 H      -3.566627     2.526898    -4.296201      19.97
 C      -4.130085     1.133950    -1.012606      36.10
 C      -4.621602    -0.191779    -0.621801      90.90
 H      -5.306665    -0.658112    -1.224757      28.26
 O      -5.203749    -0.035491     0.770884     115.90
 H      -4.426741    -0.019891     1.332751      28.61
 C      -3.485876    -1.200963    -0.542690      73.21
 H      -2.914442    -1.002177    -1.622964      24.95
 C      -3.633990    -2.542603     0.047941     133.22
 O      -4.292988    -3.485740    -0.798606     113.26
 H      -3.809453    -3.443357    -1.855262      26.65
 H      -4.251880    -2.527488     1.003542      27.06
 H      -2.755563    -3.018767    -0.060635      27.65
 C       0.983243    -1.168739    -1.114887      42.06
 H       1.355331    -1.733321    -2.018202      20.03
 C       1.167691     0.195654     0.858473     102.70
 H       1.489699     1.021641     1.386552      19.82
 C      -0.201967     0.176237     1.106418      28.42
 O      -0.889703     0.775448     2.140818     224.52
 C      -0.259110     1.434857     3.158339      95.69
 H       0.170869     2.277957     2.735703      28.03
 H      -1.107209     1.986234     4.183178      22.63
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 H       0.769144     1.012064     3.658779      26.06
 C      -1.055226    -0.549931     0.141872      21.50
 O      -2.493984    -0.408256     0.404226     105.56
 C      -0.375895    -1.211842    -0.866682      70.72
 H      -0.979928    -1.950849    -1.424066      23.84
 C       1.780312    -0.317418    -0.340774      38.03
 C       3.322218    -0.037640    -0.721301      56.19
 H       3.515440    -0.047842    -1.940501      23.80
 O       3.617074     1.369742    -0.667202     198.40
 H       3.801007     1.699955     0.256149      26.65
 C       4.249096    -0.998530     0.296997     111.22
 H       3.852985    -0.636930     1.164545      32.36
 O       3.773524    -2.246406     0.104659     295.26
 H       3.825606    -2.457418    -0.968733      26.86
 C       5.698280    -0.896844     0.100467     110.17
 O       6.419507     0.368572    -0.007541     240.72
 H       6.543249     0.857494     0.893564      28.15
 H       5.728448    -1.208345    -0.934960      32.25
 H       6.226996    -1.653683     0.703493      30.93
55
name= lig-ACN-Water-frame_713
 C      -4.104804     1.238588    -2.559590      63.14
 H      -4.177625     0.375489    -3.193079      22.94
 C      -4.003944     2.432190    -0.267615      87.34
 H      -4.183524     2.268187     0.720005      23.29
 C      -3.551472     3.554753    -0.969837      43.06
 O      -3.638290     4.707787    -0.318584     194.79
 C      -3.122580     4.775063     1.106354      91.24
 H      -2.720132     3.859308     1.421071      28.33
 H      -3.925543     5.091345     1.948737      22.72
 H      -2.182180     5.383364     0.995848      24.44
 C      -3.284588     3.601130    -2.272783      37.22
 O      -2.798645     4.740054    -3.028509     149.31
 H      -2.948582     5.463059    -2.301325      23.58
 C      -3.612788     2.499325    -3.029269      29.01
 H      -3.764001     2.631278    -4.150283      22.76
 C      -4.220360     1.270650    -1.167511     -65.33
 C      -4.687780    -0.205338    -0.506337      84.99
 H      -5.498097    -0.582247    -1.080337      26.31
 O      -5.106809    -0.093339     0.816924     130.15
 H      -4.364522     0.135781     1.482183      24.22
 C      -3.328844    -1.053799    -0.581368      81.25
 H      -2.954346    -1.388679    -1.716713      22.69
 C      -3.570366    -2.535541     0.058421     105.49
 O      -4.300739    -3.574840    -0.783964     135.59
 H      -3.964194    -3.337430    -1.842291      26.92
 H      -4.159787    -2.402947     0.993351      26.22
 H      -2.714993    -2.710953     0.608787      28.04
 C       0.973173    -1.075572    -1.156617      36.69
 H       1.489038    -1.717214    -1.854395      21.38
 C       1.198690     0.327144     0.802504      71.26
 H       1.897894     0.547353     1.502291      20.58
 C      -0.268828     0.054780     1.069253      -2.12
 O      -0.995218     0.672710     2.160076     138.11
 C      -0.162543     1.515831     3.117906      85.41
 H       0.224701     2.394597     2.805290      26.76
 H      -1.301724     1.668386     3.959411      21.12
 H       0.440459     0.684450     3.660913      24.11
 C      -1.119504    -0.496189     0.120844      23.32
 O      -2.458400    -0.528354     0.351100     208.08
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 C      -0.466459    -1.305823    -0.891831      47.81
 H      -0.928410    -1.971241    -1.712241      20.87
 C       1.768700    -0.412571    -0.206251      26.46
 C       3.177528    -0.032191    -0.642417      62.28
 H       3.144955    -0.516220    -1.771569      21.39
 O       3.628293     1.486487    -0.626701     152.68
 H       3.919563     1.572982     0.299980      25.32
 C       4.156023    -0.810532     0.273697      97.42
 H       4.089615    -0.641448     1.315153      26.11
 O       3.833985    -2.325674     0.128902     226.28
 H       3.829883    -2.593037    -0.910533      24.78
 C       5.795074    -0.938560     0.010733     100.65
 O       6.430064     0.445144     0.009956     221.40
 H       6.575167     0.676651     0.997319      28.22
 H       6.101688    -1.483218    -0.846774      32.23
 H       6.148411    -1.484463     0.852099      31.50
55
name= lig-ACN-Water-frame_714
 C      -4.018484     1.295817    -2.619319      56.00
 H      -4.171262     0.513354    -3.242309      26.46
 C      -4.034574     2.288497    -0.413100      59.75
 H      -4.058897     2.308548     0.575015      23.34
 C      -3.593030     3.572138    -0.933038     -14.53
 O      -3.600561     4.806593    -0.161512     237.56
 C      -3.090060     4.786532     1.115384     109.67
 H      -2.916628     3.832264     1.450330      27.17
 H      -3.932265     5.425463     1.780420      21.26
 H      -2.242233     5.474734     1.127067      24.95
 C      -3.193299     3.640290    -2.410173     -10.36
 O      -2.813448     4.768634    -3.054294     188.14
 H      -2.619157     5.620447    -2.536803      21.37
 C      -3.600171     2.509160    -3.222241      43.87
 H      -3.265439     2.641998    -4.239776      22.90
 C      -4.389123     1.187146    -1.152457      67.46
 C      -4.558234    -0.080539    -0.473745     100.68
 H      -5.356735    -0.663312    -0.970708      25.27
 O      -5.077227    -0.135254     0.926763     165.34
 H      -4.246243    -0.058576     1.595030      22.95
 C      -3.376013    -1.154212    -0.579942      64.09
 H      -2.878903    -0.828464    -1.677446      22.65
 C      -3.585466    -2.543909     0.082507     121.44
 O      -4.243576    -3.586016    -0.757334     229.52
 H      -4.104870    -3.331848    -1.639354      33.77
 H      -4.379001    -2.313654     0.752754      27.23
 H      -2.746279    -3.033204     0.359354      29.36
 C       0.887613    -1.126149    -1.128682      30.85
 H       1.277528    -1.448738    -2.048312      21.84
 C       1.064612     0.327788     0.947332     100.66
 H       1.597189     0.803747     1.737233      20.45
 C      -0.258139     0.154685     1.065277      24.87
 O      -0.960067     0.616925     2.136067     224.18
 C      -0.224618     1.423818     3.101303     100.53
 H       0.261999     2.104834     2.548875      26.84
 H      -0.989331     2.161866     4.029148      21.31
 H       0.607841     0.932897     3.692925      25.47
 C      -1.037832    -0.616351     0.035908      24.34
 O      -2.367493    -0.554186     0.313997     170.82
 C      -0.462252    -1.304866    -0.994863      43.47
 H      -1.244826    -1.811463    -1.675283      17.52
 C       1.726657    -0.315466    -0.262537      65.70
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 C       3.188720    -0.009332    -0.539755      83.10
 H       3.547705    -0.254653    -1.670763      23.73
 O       3.538614     1.463205    -0.574279     188.59
 H       4.048734     1.721806     0.237045      24.57
 C       4.226146    -0.883361     0.196997     104.18
 H       4.054496    -0.554901     1.240994      24.92
 O       3.872124    -2.334575     0.204792     282.01
 H       4.211308    -2.642391    -0.670639      29.91
 C       5.827349    -0.805866    -0.018957     115.16
 O       6.445691     0.436928     0.025830     307.91
 H       6.591810     0.767241     0.901980      31.58
 H       6.160954    -1.271446    -0.899573      31.25
 H       6.091172    -1.379695     0.794755      31.16
55
name= lig-ACN-Water-frame_715
 C      -4.037500     1.351546    -2.635419      48.46
 H      -4.302746     0.574336    -3.207317      28.57
 C      -4.049810     2.356300    -0.478292      40.02
 H      -4.327736     2.223403     0.501594      21.15
 C      -3.606010     3.536424    -1.057528       7.85
 O      -3.598870     4.866857    -0.187003     133.40
 C      -3.015385     4.858696     1.260067     101.96
 H      -3.012172     3.906271     1.710668      26.59
 H      -3.905543     5.409846     1.958519      22.74
 H      -2.081194     5.286149     1.317080      27.02
 C      -3.302919     3.653433    -2.396672      -4.42
 O      -2.816193     4.836803    -3.064634     230.72
 H      -2.774482     5.470170    -2.332843      24.19
 C      -3.484670     2.510155    -3.289636      50.32
 H      -3.192004     2.320643    -4.230625      24.92
 C      -4.301079     1.182281    -1.290684     -30.21
 C      -4.569255    -0.262926    -0.436089      78.64
 H      -5.377785    -0.734305    -1.057991      27.27
 O      -5.054863    -0.113959     0.957676     131.53
 H      -4.255049    -0.001303     1.678568      18.86
 C      -3.352612    -1.137776    -0.535299      93.69
 H      -3.190354    -1.471488    -1.689720      24.51
 C      -3.675162    -2.570232     0.041195     131.87
 O      -4.230951    -3.584915    -0.782688     247.42
 H      -3.972170    -3.397607    -1.637167      34.47
 H      -4.026228    -2.600471     1.010393      28.36
 H      -2.687012    -2.744398     0.312179      28.56
 C       1.005547    -1.106422    -1.167635      38.69
 H       1.537606    -1.446180    -2.018059      20.54
 C       1.142147     0.221781     0.940554      67.62
 H       1.642147     1.118447     1.492280      18.01
 C      -0.338741     0.174070     0.992020       4.69
 O      -0.970489     0.605496     2.206338     163.75
 C      -0.202668     1.399817     3.044337     104.35
 H       0.294428     2.219049     2.610272      26.35
 H      -1.238566     1.988113     3.760593      21.65
 H       0.417711     0.786221     3.656506      26.90
 C      -1.009666    -0.667978     0.113073      29.29
 O      -2.337909    -0.546378     0.304262     179.23
 C      -0.462167    -1.247454    -1.055353      59.94
 H      -0.882904    -1.917429    -1.861919      22.38
 C       1.622705    -0.199516    -0.281578      10.05
 C       3.294816    -0.004272    -0.658827      59.18
 H       3.130252    -0.206686    -1.791478      24.24
 O       3.443923     1.405293    -0.517328     199.75
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 H       3.493751     1.582045     0.519884      21.65
 C       4.322678    -0.971469     0.315276      86.77
 H       4.106596    -0.709883     1.411547      25.93
 O       3.948228    -2.298235     0.254843     330.47
 H       3.914695    -2.687834    -0.598036      30.63
 C       5.780863    -0.790967    -0.011027     111.55
 O       6.507395     0.532983     0.017836     274.05
 H       6.514522     0.878390     0.947289      29.74
 H       5.840395    -1.024711    -1.035378      30.41
 H       6.363473    -1.496120     0.480231      31.06
55
name= lig-ACN-Water-frame_716
 C      -4.078338     1.270169    -2.744982      57.68
 H      -4.112486     0.494135    -3.459486      23.15
 C      -4.110983     2.400711    -0.479997      70.81
 H      -4.391478     2.473005     0.583615      24.06
 C      -3.630653     3.686936    -1.006055       0.71
 O      -3.558125     4.789243    -0.277370     124.29
 C      -3.033442     4.864371     1.309483      71.00
 H      -2.984140     3.813818     1.642254      24.88
 H      -3.645601     5.747862     1.921334      22.31
 H      -2.131096     5.210781     1.120238      27.81
 C      -3.366888     3.714719    -2.529975       9.67
 O      -2.851380     4.864469    -2.977434     189.97
 H      -3.139067     5.654110    -2.483218      24.45
 C      -3.411281     2.473797    -3.185239      57.96
 H      -3.275203     2.739027    -4.131600      25.97
 C      -4.158722     1.199276    -1.245455      -8.59
 C      -4.660262    -0.271489    -0.490745      88.21
 H      -5.574449    -0.880571    -0.896618      24.52
 O      -5.080979    -0.061915     0.833820     171.27
 H      -4.318778     0.137935     1.493197      23.50
 C      -3.424375    -1.225420    -0.464615      95.25
 H      -2.858649    -1.154827    -1.516924      23.84
 C      -3.536435    -2.639989     0.131034     117.57
 O      -4.284757    -3.569176    -0.861273     145.41
 H      -3.732744    -3.490196    -1.809034      27.05
 H      -4.238626    -2.631713     0.871523      28.44
 H      -2.647236    -3.152709     0.310666      27.28
 C       1.039403    -1.001334    -1.229815      55.91
 H       1.521298    -1.680270    -1.920244      26.71
 C       1.098763     0.268618     0.823687      87.71
 H       1.893368     0.786636     1.598574      18.98
 C      -0.228224     0.078454     1.087105      15.60
 O      -1.003483     0.564729     2.127702     183.83
 C      -0.216985     1.441375     3.107081      98.75
 H       0.432882     2.192040     2.570373      24.82
 H      -1.064013     1.907619     3.965535      23.94
 H       0.365575     0.848601     3.706795      28.18
 C      -1.041087    -0.661737     0.058567       2.83
 O      -2.439752    -0.546820     0.298426     132.07
 C      -0.297963    -1.216337    -1.043484      74.50
 H      -0.930570    -1.797096    -1.676803      22.75
 C       1.873759    -0.316178    -0.378131      37.60
 C       3.195480    -0.061770    -0.640922      96.18
 H       3.733909    -0.409985    -1.534110      23.19
 O       3.411129     1.395294    -0.485618     176.83
 H       3.614464     1.523205     0.553438      21.57
 C       4.244059    -0.840946     0.395339      87.31
 H       4.116099    -0.597776     1.538245      25.00
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 O       4.007674    -2.375386     0.285264     266.89
 H       3.966662    -2.411325    -0.708589      26.43
 C       5.878700    -0.766995    -0.102841      96.99
 O       6.507041     0.601533     0.007943     227.51
 H       6.642194     0.927697     1.002829      27.39
 H       5.804794    -0.965919    -1.166141      31.81
 H       6.435059    -1.500332     0.323022      32.40
55
name= lig-ACN-Water-frame_717
55
name= lig-ACN-Water-frame_718
 C      -3.742241     1.332777    -2.537220      66.75
 H      -3.757025     0.436045    -3.331022      23.78
 C      -4.165297     2.282392    -0.396988      64.53
 H      -4.402666     2.125501     0.764504      18.66
 C      -3.740165     3.597711    -0.952013      -5.83
 O      -3.511965     4.791947    -0.354593     210.94
 C      -3.089312     4.837879     1.044499     103.77
 H      -3.375706     3.740146     1.416210      22.32
 H      -3.532735     5.747046     1.599504      23.68
 H      -2.017217     4.874253     0.995345      28.23
 C      -3.362269     3.715551    -2.441411      -3.59
 O      -2.965165     4.901548    -2.956656     168.09
 H      -3.231336     5.648103    -2.307236      21.09
 C      -3.609785     2.549267    -3.149368      61.51
 H      -3.267201     2.710852    -4.187272      22.95
 C      -4.235076     1.217044    -1.258207      63.60
 C      -4.552677    -0.172714    -0.664467      82.73
 H      -5.483086    -0.796733    -1.151703      23.56
 O      -5.320434     0.122408     0.616455      89.04
 H      -4.719044     0.160197     1.381502      26.74
 C      -3.347611    -1.247761    -0.504273      76.21
 H      -2.731211    -1.419947    -1.396188      23.62
 C      -3.638605    -2.762926     0.034757     115.86
 O      -4.347583    -3.491965    -0.968800     179.91
 H      -3.899916    -3.241788    -1.960125      25.80
 H      -4.211235    -3.079917     0.896585      25.57
 H      -2.651414    -3.124726    -0.049783      26.25
 C       0.981724    -1.168742    -1.265375      44.83
 H       1.441874    -1.437590    -2.295894      16.74
 C       1.223182     0.117993     0.836233      70.99
 H       1.943807     0.942017     1.168784      12.46
 C      -0.157457     0.100834     1.025127      26.95
 O      -0.812978     0.570302     2.072538     217.64
 C      -0.295075     1.330703     3.128725     129.29
 H       0.306415     2.349871     2.894854      25.12
 H      -1.202242     1.296378     3.664434      25.64
 H       0.236919     0.779900     3.729817      30.48
 C      -1.005962    -0.590120     0.061264       0.84
 O      -2.362045    -0.561830     0.327866     157.07
 C      -0.412351    -1.236452    -1.127966      72.30
 H      -1.093270    -1.641214    -1.754490      24.65
 C       1.894472    -0.465867    -0.346891      32.92
 C       3.330876    -0.095491    -0.557660      87.84
 H       3.693205    -0.444587    -1.492557      25.01
 O       3.550960     1.367560    -0.511916     148.17
 H       3.562409     1.590733     0.442910      25.94
 C       4.451300    -0.913852     0.382345      97.15
 H       4.462319    -0.620877     1.547582      25.98
 O       4.115235    -2.281968     0.302409     265.13
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 H       4.155436    -2.441294    -0.748277      25.86
 C       5.850347    -0.682317    -0.013948     109.54
 O       6.460168     0.694203    -0.096193     304.07
 H       6.523626     1.136476     0.765627      31.70
 H       5.876446    -1.074806    -1.100731      30.46
 H       6.463899    -1.258941     0.508282      32.08
55
name= lig-ACN-Water-frame_719
 C      -3.717794     1.321016    -2.596161      31.79
 H      -3.478167     0.283618    -3.232784      23.16
 C      -4.138210     2.426926    -0.318256      43.32
 H      -4.557022     2.451470     0.786094      21.05
 C      -3.696818     3.507712    -1.001968      29.13
 O      -3.568255     4.812979    -0.443447     194.05
 C      -3.084314     4.779257     1.051793     105.75
 H      -3.499291     3.924345     1.809333      22.93
 H      -3.489132     5.688149     1.482466      25.52
 H      -1.961810     4.821830     1.049065      26.11
 C      -3.488837     3.669597    -2.338124      22.33
 O      -3.059722     4.878573    -2.947396     183.61
 H      -2.970205     5.595692    -2.309568      22.81
 C      -3.525994     2.626769    -3.217599      44.11
 H      -3.580258     2.604403    -4.379461      23.50
 C      -4.141395     1.146090    -1.203575     -47.15
 C      -4.556980    -0.246578    -0.614315      84.49
 H      -5.116024    -0.874622    -1.530282      25.95
 O      -5.402903     0.125967     0.505478     150.95
 H      -4.747851     0.199835     1.292249      26.08
 C      -3.345003    -1.127766    -0.430929     107.78
 H      -3.190107    -1.146989    -1.562830      24.76
 C      -3.629299    -2.633849    -0.106346     113.19
 O      -4.461883    -3.493719    -1.080427     206.14
 H      -4.049956    -3.329233    -1.952023      29.31
 H      -4.072774    -2.509977     0.939526      25.62
 H      -2.709104    -3.119492     0.149509      27.24
 C       0.992543    -1.199740    -1.208578      47.59
 H       1.442240    -1.908831    -2.006092      19.71
 C       1.297494     0.049696     0.859463      83.26
 H       1.681559     0.741755     1.602907      17.70
 C      -0.094847     0.134671     0.882758      11.35
 O      -0.840629     0.568809     2.042877     177.37
 C      -0.298644     1.245535     3.250686     129.79
 H       0.056419     2.331556     2.944756      25.44
 H      -0.940180     1.703929     3.862405      27.35
 H       0.484551     0.763179     3.618627      29.05
 C      -0.946846    -0.687300     0.022926      19.67
 O      -2.298108    -0.606412     0.359729     190.31
 C      -0.427418    -1.238788    -1.086248      73.96
 H      -0.833127    -1.847737    -1.848287      23.36
 C       1.819369    -0.508747    -0.338612      26.35
 C       3.342760    -0.156053    -0.627592      84.86
 H       3.543358    -0.330244    -1.613949      25.66
 O       3.594231     1.294683    -0.467133     174.31
 H       3.695452     1.553041     0.478827      25.43
 C       4.385925    -0.804699     0.458325      76.83
 H       4.040972    -0.546224     1.567236      24.85
 O       4.186987    -2.308416     0.285495     285.47
 H       3.948494    -2.520062    -0.649555      27.38
 C       6.077560    -0.699401    -0.016814      94.68
 O       6.388240     0.729348    -0.180699     258.59
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 H       6.483581     1.056219     0.742383      29.14
 H       6.209527    -1.126262    -1.047125      30.87
 H       6.592274    -1.286425     0.622868      32.49
55
name= lig-ACN-Water-frame_720
 C      -3.764279     1.299974    -2.565667      54.30
 H      -3.894557     0.289296    -3.266611      21.14
 C      -4.123560     2.331967    -0.457339      75.77
 H      -4.459932     2.399420     0.613196      23.55
 C      -3.666893     3.617237    -0.984574       3.74
 O      -3.605440     4.800996    -0.285240     272.56
 C      -3.105235     4.813223     0.967498     130.28
 H      -3.708346     4.070279     1.577389      25.56
 H      -3.323132     5.802817     1.267487      24.78
 H      -1.954578     4.528236     1.109796      26.96
 C      -3.511311     3.682417    -2.433314       0.77
 O      -3.168165     4.879853    -2.938544     150.47
 H      -3.241177     5.552852    -2.231011      23.77
 C      -3.486683     2.457413    -3.243726      47.78
 H      -3.276691     2.730877    -4.400989      22.83
 C      -3.987628     1.212242    -1.170395      48.43
 C      -4.544272    -0.107293    -0.611223      82.15
 H      -5.396391    -0.571010    -1.392824      22.16
 O      -5.472332     0.034978     0.471240     106.97
 H      -4.997498     0.336006     1.317432      26.02
 C      -3.324776    -1.131815    -0.586841      72.08
 H      -2.761175    -1.057804    -1.600084      21.30
 C      -3.661556    -2.568973    -0.171918     109.10
 O      -4.524199    -3.368452    -1.105830     239.74
 H      -4.118354    -3.489483    -1.870675      34.11
 H      -4.463029    -2.674036     0.653347      22.95
 H      -2.720209    -3.129744     0.022405      25.40
 C       1.087854    -1.272870    -1.231280      44.46
 H       1.597468    -1.865289    -2.068210      24.33
 C       1.281048     0.117758     0.849681      91.36
 H       1.965582     0.078921     1.588741      20.37
 C      -0.172388     0.025583     0.988311       6.42
 O      -0.919540     0.604920     2.046394     168.91
 C      -0.215222     1.206936     3.241321     121.76
 H       0.288099     2.086238     2.774766      26.78
 H      -0.990088     1.181542     3.852679      28.36
 H       0.434884     0.602612     3.739931      30.05
 C      -0.960168    -0.621775     0.039917       6.41
 O      -2.293515    -0.634010     0.448504     151.82
 C      -0.337738    -1.374467    -1.076884      62.47
 H      -1.092872    -2.027832    -1.595912      19.04
 C       1.923434    -0.491428    -0.282544      19.38
 C       3.435874    -0.181547    -0.553711     110.33
 H       3.602542    -0.434722    -1.504325      28.86
 O       3.542603     1.239908    -0.407578     160.85
 H       3.993993     1.366849     0.485666      26.85
 C       4.411925    -0.961287     0.249396     114.54
 H       4.202389    -0.576487     1.330165      27.56
 O       4.234969    -2.313861     0.346913     292.53
 H       4.362452    -2.588527    -0.559168      31.17
 C       6.019431    -0.615346     0.022092     110.16
 O       6.392295     0.718173    -0.253028     216.82
 H       6.587898     1.284275     0.594692      25.88
 H       6.237154    -1.252837    -0.834360      32.52
 H       6.662517    -0.851719     0.787313      32.29
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55
name= lig-ACN-Water-frame_721
 C      -3.801874     1.200288    -2.618624      80.28
 H      -4.126490     0.257930    -3.260174      22.70
 C      -4.013320     2.420644    -0.467987      79.68
 H      -4.261632     2.220346     0.526150      22.95
 C      -3.723079     3.603741    -1.054113      14.36
 O      -3.695447     4.801809    -0.316464     273.19
 C      -3.095935     4.860633     1.103913     111.77
 H      -3.628940     4.290085     1.857891      26.69
 H      -3.010202     5.824624     1.453275      26.02
 H      -2.079130     4.409019     0.894504      27.83
 C      -3.426358     3.642754    -2.455937      22.03
 O      -3.277097     4.949737    -3.003596     162.40
 H      -3.363212     5.682029    -2.276786      22.58
 C      -3.474164     2.469121    -3.170003      59.72
 H      -3.098916     2.245240    -4.272325      21.14
 C      -3.994150     1.235593    -1.238737      27.92
 C      -4.504175    -0.041347    -0.724931      61.93
 H      -5.209025    -0.478474    -1.634167      21.44
 O      -5.463677    -0.024468     0.523393     133.80
 H      -4.995745     0.299809     1.300367      27.76
 C      -3.303319    -1.127700    -0.641543      68.46
 H      -2.781507    -1.127997    -1.628801      20.06
 C      -3.773941    -2.596723    -0.217470     109.67
 O      -4.582317    -3.211465    -1.146513     277.69
 H      -3.942599    -3.299081    -1.931723      27.23
 H      -4.110002    -2.403984     0.892914      24.03
 H      -2.787561    -3.164116    -0.043269      23.58
 C       1.192335    -1.295534    -1.198229      50.29
 H       1.636281    -1.599479    -2.155503      21.90
 C       1.229526     0.060842     0.887695      69.10
 H       1.693280     0.608475     1.580679      19.16
 C      -0.142686    -0.013382     1.140629      17.38
 O      -0.934501     0.619658     2.078052     218.57
 C      -0.172408     1.089414     3.165240     140.55
 H       0.271907     2.042140     3.223259      27.49
 H      -0.804405     1.430293     3.902130      26.67
 H       0.537826     0.331117     3.356608      29.02
 C      -0.922125    -0.635984     0.026598      15.45
 O      -2.393963    -0.694365     0.427303     155.88
 C      -0.265671    -1.423704    -0.906341      70.01
 H      -0.737400    -2.123287    -1.737148      19.81
 C       1.929493    -0.562325    -0.327211      21.67
 C       3.396113    -0.222746    -0.593755      93.15
 H       3.595590    -0.280335    -1.565425      25.18
 O       3.541820     1.236133    -0.337572     217.77
 H       3.695343     1.509130     0.635081      22.61
 C       4.541292    -0.962489     0.298061      88.45
 H       4.376506    -0.668166     1.389503      24.35
 O       4.294372    -2.439223     0.362331     253.55
 H       4.407384    -2.895890    -0.507567      28.62
 C       5.946517    -0.622929     0.025856     111.80
 O       6.424683     0.784436    -0.365213     261.28
 H       6.367212     1.293547     0.530392      28.45
 H       6.454493    -1.155277    -0.712930      29.91
 H       6.245380    -1.032376     0.978746      29.96
55
name= lig-ACN-Water-frame_722
 C      -3.828162     1.270853    -2.659821      46.47
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 H      -3.793268     0.367005    -3.297295      22.20
 C      -3.886672     2.377631    -0.395492      39.42
 H      -4.033604     2.531704     0.616617      19.20
 C      -3.717546     3.654186    -1.056435      -5.00
 O      -3.804424     4.867489    -0.356191     166.49
 C      -3.054459     4.843296     1.155410      88.37
 H      -3.722241     4.550739     1.824540      26.08
 H      -2.883976     5.865101     1.134624      25.73
 H      -2.064487     4.169583     1.249706      24.08
 C      -3.382460     3.741140    -2.425686      -2.21
 O      -3.363967     4.962800    -3.119165     179.38
 H      -3.171547     5.682453    -2.405622      22.53
 C      -3.400917     2.473773    -3.246611      34.33
 H      -3.315532     2.760251    -4.352364      24.78
 C      -4.148702     1.206750    -1.269929      23.57
 C      -4.521887    -0.194093    -0.712220      94.91
 H      -5.291286    -0.723100    -1.470181      23.44
 O      -5.317071    -0.030256     0.478368     193.89
 H      -4.688507     0.108424     1.222881      25.17
 C      -3.377285    -1.143211    -0.604774      96.56
 H      -3.028462    -1.230753    -1.620063      25.03
 C      -3.722465    -2.505813    -0.180401     103.63
 O      -4.692887    -3.096744    -1.215823      88.65
 H      -4.265024    -3.163222    -2.294340      23.35
 H      -4.478675    -2.615806     0.713770      23.94
 H      -2.805079    -3.231608    -0.100358      24.86
 C       1.141957    -1.296282    -1.127483      50.11
 H       1.458083    -1.780041    -2.013758      22.87
 C       1.302029     0.002095     0.917409     123.00
 H       1.674254     0.878796     1.146152      15.59
 C      -0.203767    -0.056396     1.008294      22.00
 O      -0.899374     0.631218     2.057944     206.42
 C      -0.102300     1.023735     3.262193      97.68
 H       0.420256     1.739001     2.767669      26.07
 H      -0.747214     1.102086     4.076357      27.49
 H       0.569454     0.240837     3.622176      28.32
 C      -0.983226    -0.790031     0.208920      26.43
 O      -2.326472    -0.730517     0.300545     202.28
 C      -0.205564    -1.427932    -0.849009      59.88
 H      -0.987413    -1.900321    -1.640797      19.21
 C       1.908580    -0.547590    -0.164600      38.46
 C       3.392517    -0.186534    -0.541294      96.02
 H       3.514287    -0.406322    -1.522129      27.39
 O       3.548917     1.258704    -0.303614     224.25
 H       3.554083     1.327315     0.676137      26.07
 C       4.382971    -0.955491     0.370963      80.18
 H       4.066371    -0.661267     1.371230      28.05
 O       4.396559    -2.529809     0.368704     216.50
 H       4.177392    -2.546475    -0.638338      26.81
 C       6.109957    -0.623446    -0.030211      91.00
 O       6.387666     0.749276    -0.389466     275.56
 H       6.364893     1.307877     0.381331      30.33
 H       6.251574    -1.281771    -0.823664      31.75
 H       6.900001    -0.752945     0.757649      29.00
55
name= lig-ACN-Water-frame_723
 C      -3.817058     1.422137    -2.658274      58.68
 H      -3.901165     0.605828    -3.280927      23.71
 C      -3.884502     2.334364    -0.469573      53.03
 H      -3.954223     2.062393     0.564955      22.64
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 C      -3.633192     3.655547    -1.014454     -20.45
 O      -3.781264     4.873615    -0.247534     231.81
 C      -3.129213     4.899196     1.007091     119.74
 H      -3.800002     4.765096     1.715265      27.86
 H      -2.593794     5.828179     1.267862      26.28
 H      -2.340186     3.978450     1.070884      24.77
 C      -3.445990     3.759665    -2.498628      11.06
 O      -3.398552     4.945446    -3.204588     157.05
 H      -3.355827     5.744203    -2.675857      27.70
 C      -3.385132     2.669638    -3.257897      70.63
 H      -3.295506     2.662057    -4.320842      28.37
 C      -4.175624     1.202675    -1.280740      13.54
 C      -4.570233    -0.204929    -0.725001      95.81
 H      -5.306792    -0.792489    -1.408501      24.75
 O      -5.196591    -0.065087     0.517500     185.64
 H      -4.618824     0.306001     1.307872      22.13
 C      -3.312627    -1.201684    -0.671588      85.61
 H      -2.898036    -1.255617    -1.606006      26.91
 C      -3.855986    -2.629964    -0.241156     103.43
 O      -4.774976    -2.979620    -1.244883     120.95
 H      -4.021772    -3.264948    -2.178813      21.31
 H      -4.325185    -2.602132     0.849580      24.83
 H      -2.829887    -3.255568    -0.127608      24.90
 C       1.084106    -1.326764    -0.991020      45.47
 H       1.645424    -1.793283    -1.740647      24.01
 C       1.196697     0.101050     0.938467      78.55
 H       1.777642     0.592793     1.669609      22.54
 C      -0.138315    -0.014583     1.110545      23.43
 O      -0.850781     0.594919     2.075863     186.97
 C      -0.002574     0.958882     3.276519     117.02
 H       0.518945     1.805953     3.402733      27.46
 H      -0.822819     1.322525     3.860463      26.29
 H       0.607221     0.037120     3.526399      26.63
 C      -0.945663    -0.988020     0.218911      32.11
 O      -2.315573    -0.683670     0.295136     152.58
 C      -0.355846    -1.462603    -0.919631      92.80
 H      -0.855170    -2.118641    -1.747265      21.69
 C       1.944012    -0.602607    -0.163452      38.20
 C       3.350814    -0.187391    -0.417180      92.66
 H       3.602433    -0.313642    -1.429384      25.53
 O       3.549809     1.252060    -0.293186     238.49
 H       4.016323     1.538820     0.498492      29.21
 C       4.479489    -1.040601     0.457204      99.20
 H       4.398936    -0.861464     1.490397      29.12
 O       4.434097    -2.428606     0.318114     264.84
 H       4.264308    -2.887213    -0.559663      28.51
 C       6.073157    -0.623678    -0.040544      99.04
 O       6.324253     0.719136    -0.433977     185.01
 H       6.550078     1.164245     0.402769      29.38
 H       6.153725    -1.093040    -0.965233      33.12
 H       6.828206    -1.239490     0.653464      30.87
55
name= lig-ACN-Water-frame_724
 C      -3.844461     1.445240    -2.732543      56.86
 H      -3.994896     0.708731    -3.352188      25.62
 C      -3.940021     2.370673    -0.514500      64.40
 H      -4.014633     2.425904     0.633283      23.03
 C      -3.607628     3.637632    -1.027777      -9.84
 O      -3.742883     4.829948    -0.304729     204.92
 C      -3.155967     4.919385     1.035697     108.26
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 H      -3.837311     4.966957     1.773656      26.64
 H      -2.440921     5.774331     0.883002      24.25
 H      -2.489669     3.879451     1.164351      22.85
 C      -3.519040     3.879052    -2.407668       0.50
 O      -3.407111     5.017443    -3.261869     166.84
 H      -3.571221     5.784120    -2.683681      27.21
 C      -3.471594     2.655911    -3.244070      35.27
 H      -3.142220     2.717870    -4.187493      26.41
 C      -4.051806     1.253615    -1.379480      28.67
 C      -4.446193    -0.125732    -0.792660      62.67
 H      -5.237929    -0.450062    -1.472520      26.02
 O      -5.205049    -0.126341     0.607105      97.80
 H      -4.524950     0.237424     1.326100      23.44
 C      -3.245867    -1.237543    -0.688353      88.76
 H      -2.812152    -1.297581    -1.600343      26.52
 C      -3.861468    -2.665880    -0.268431     104.35
 O      -4.825760    -2.956842    -1.322766      81.18
 H      -4.201300    -3.347215    -2.259021      23.81
 H      -4.456375    -2.506193     0.705506      24.61
 H      -3.207381    -3.694824    -0.259409      24.21
 C       1.109310    -1.434667    -0.991347      43.03
 H       1.535269    -1.835845    -1.874804      20.95
 C       1.277657     0.147564     0.938944      86.13
 H       1.805350     0.563795     1.862587      20.20
 C      -0.195528    -0.168968     1.114198      25.31
 O      -0.779322     0.618526     2.176328     220.92
 C      -0.045754     0.921662     3.330199     130.97
 H       0.660578     1.584800     3.046389      27.79
 H      -0.660648     1.042484     4.194557      25.90
 H       0.413080    -0.071038     3.765082      26.91
 C      -0.965864    -0.855936     0.199667      16.17
 O      -2.376354    -0.657440     0.352391     198.42
 C      -0.310826    -1.554683    -0.961441      64.25
 H      -0.901339    -2.050032    -1.746114      18.51
 C       1.804954    -0.545740    -0.046075      36.02
 C       3.458594    -0.259148    -0.297630      69.60
 H       3.575310    -0.639915    -1.315916      25.14
 O       3.539231     1.251226    -0.294028     203.25
 H       3.784783     1.459163     0.672342      25.50
 C       4.637652    -0.976103     0.480436     114.35
 H       4.630293    -0.782913     1.476130      30.44
 O       4.424862    -2.415897     0.284536     247.46
 H       4.415322    -2.408567    -0.668103      30.84
 C       5.889374    -0.749177    -0.148354     103.93
 O       6.300207     0.734472    -0.389857     186.10
 H       6.546100     1.286295     0.455432      27.64
 H       6.006524    -1.272419    -1.078794      32.16
 H       6.708483    -1.078180     0.672814      28.88
55
name= lig-ACN-Water-frame_725
 C      -3.872442     1.350819    -2.810343      48.25
 H      -3.691705     0.512780    -3.399126      21.52
 C      -3.932549     2.459583    -0.518942      65.68
 H      -4.357634     2.268970     0.598472      23.44
 C      -3.698625     3.730770    -1.095147      22.52
 O      -3.738663     4.843001    -0.370404     166.37
 C      -3.087915     4.895179     1.086435      90.21
 H      -3.890903     5.238331     1.647493      24.75
 H      -2.402627     5.849317     1.077454      24.59
 H      -2.533036     3.950695     1.679432      23.43
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 C      -3.518546     3.858074    -2.538247      19.81
 O      -3.422264     5.116694    -3.198311     169.99
 H      -3.317063     5.968086    -2.606928      23.18
 C      -3.558031     2.727297    -3.279930      48.08
 H      -3.450140     2.995262    -4.234602      27.84
 C      -3.955395     1.267783    -1.283333      -4.59
 C      -4.374222    -0.135464    -0.725510      96.20
 H      -5.030682    -0.592695    -1.391148      26.84
 O      -5.189018    -0.171171     0.481246     158.49
 H      -4.690868     0.128054     1.291520      26.44
 C      -3.281134    -1.210418    -0.650777      96.12
 H      -2.755941    -1.289494    -1.530147      27.10
 C      -3.876072    -2.615761    -0.354040      99.93
 O      -4.864015    -2.979422    -1.440806     155.02
 H      -4.287820    -3.149366    -2.317719      26.72
 H      -4.562498    -2.603233     0.529815      25.31
 H      -2.870103    -3.276487    -0.063459      23.98
 C       1.161874    -1.419373    -0.982391      50.38
 H       1.716496    -1.955856    -1.762815      22.26
 C       1.153514     0.002608     1.039422      61.25
 H       1.820188     0.919847     1.417802      18.63
 C      -0.167953    -0.094592     1.221300      14.96
 O      -0.871724     0.559248     2.203216     177.38
 C      -0.009353     0.823326     3.458318     112.96
 H       0.631270     1.592837     3.389040      28.97
 H      -0.670425     1.477834     4.020252      25.92
 H       0.703215    -0.091796     3.736381      25.91
 C      -1.017972    -0.700113     0.081099      18.06
 O      -2.365329    -0.704653     0.380046     181.11
 C      -0.270974    -1.491079    -0.782630      73.32
 H      -0.784016    -1.966243    -1.543247      24.19
 C       1.965002    -0.644134    -0.108061      19.94
 C       3.372170    -0.261116    -0.265443      94.46
 H       3.698881    -0.459207    -1.335733      21.86
 O       3.540704     1.172062    -0.298053     224.95
 H       3.460965     1.592204     0.632094      24.93
 C       4.515334    -0.930672     0.505130      95.06
 H       4.573944    -0.719626     1.484903      28.31
 O       4.397383    -2.427925     0.276817     296.71
 H       4.301669    -2.771117    -0.596730      29.17
 C       6.004326    -0.656731    -0.247528      80.33
 O       6.262749     0.682275    -0.348614     243.00
 H       6.358128     0.972736     0.613322      27.67
 H       5.905281    -1.070873    -1.294322      28.63
 H       6.892034    -1.371754     0.282948      28.03
55
name= lig-ACN-Water-frame_726
 C      -3.749697     1.447241    -2.673902      38.57
 H      -3.852043     0.530807    -3.321431      23.73
 C      -3.959018     2.447631    -0.590023      47.45
 H      -4.177531     2.574633     0.614415      18.74
 C      -3.777454     3.739787    -1.156138     -12.43
 O      -3.651966     4.957918    -0.266978     259.12
 C      -3.134913     4.979739     1.048857      85.83
 H      -3.902150     5.236740     1.826788      22.41
 H      -2.114517     5.560500     1.080600      23.01
 H      -2.840603     3.765112     1.223105      22.51
 C      -3.553646     3.903430    -2.572218      -8.90
 O      -3.417151     5.172929    -3.110713     203.39
 H      -3.228102     5.799056    -2.290292      20.48
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 C      -3.693883     2.643249    -3.441562      32.81
 H      -3.778573     2.478161    -4.473364      22.66
 C      -3.934520     1.257151    -1.342793      45.93
 C      -4.391202    -0.158529    -0.773476     105.02
 H      -4.957994    -0.488889    -1.534191      28.31
 O      -5.202608    -0.167829     0.383918     217.85
 H      -4.779771     0.357955     1.064787      27.55
 C      -3.284190    -1.140476    -0.655658      96.11
 H      -2.891920    -1.110741    -1.631936      24.57
 C      -3.945777    -2.542204    -0.426155     109.87
 O      -4.758570    -2.988301    -1.515937     215.93
 H      -4.188833    -3.219811    -2.273720      29.02
 H      -4.397312    -2.603886     0.577121      25.04
 H      -3.092309    -3.428349    -0.536910      21.76
 C       1.171877    -1.389467    -0.925341      52.45
 H       1.523708    -2.044500    -1.768263      22.02
 C       1.246969    -0.135957     0.991483      94.08
 H       1.668098     0.643362     1.822581      15.36
 C      -0.260534     0.027417     1.148472      25.89
 O      -0.920857     0.492198     2.324275     193.27
 C      -0.016714     0.858292     3.496242     105.14
 H       0.771215     1.432540     3.283418      28.06
 H      -0.807968     0.871324     4.283946      24.29
 H       0.137914    -0.272621     3.933261      24.17
 C      -0.925938    -0.615089     0.240926      24.52
 O      -2.326203    -0.796391     0.404373     189.84
 C      -0.221035    -1.387945    -0.762466      50.27
 H      -0.743920    -2.096651    -1.261764      21.82
 C       1.923007    -0.696722     0.022587      36.56
 C       3.379666    -0.245556    -0.401420      71.19
 H       3.385501    -0.565195    -1.537201      25.32
 O       3.504450     1.188640    -0.303092     196.77
 H       3.867565     1.345135     0.643761      23.17
 C       4.542431    -1.075953     0.381440     111.46
 H       4.412623    -0.856413     1.354496      30.45
 O       4.336194    -2.445398     0.366786     292.79
 H       4.337942    -2.607125    -0.636788      29.30
 C       5.923962    -0.688876    -0.282708      83.80
 O       6.305246     0.741677    -0.290431     229.11
 H       6.565187     1.194801     0.514168      27.30
 H       5.778583    -0.883038    -1.430966      28.60
 H       6.819466    -1.436435     0.157606      28.19
55
name= lig-ACN-Water-frame_727
 C      -3.690352     1.459757    -2.719278      41.06
 H      -3.940301     0.510688    -3.404412      22.61
 C      -3.998825     2.514233    -0.566748      77.21
 H      -4.034531     2.321912     0.618710      23.12
 C      -3.737620     3.770230    -1.141085      -5.93
 O      -3.635414     5.037911    -0.368159     194.37
 C      -3.141025     4.894004     1.029740      93.82
 H      -3.803035     5.467504     1.725252      24.19
 H      -2.130537     5.545310     1.086031      24.78
 H      -2.927198     3.765675     1.501547      24.10
 C      -3.676671     3.870226    -2.601168       8.05
 O      -3.383894     5.141700    -3.062192     104.87
 H      -3.564636     5.959463    -2.468157      19.77
 C      -3.764287     2.712227    -3.362988      55.08
 H      -3.644879     2.826705    -4.506799      22.47
 C      -3.971043     1.324856    -1.300114      20.54
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 C      -4.423715    -0.065462    -0.924469      85.29
 H      -5.028655    -0.511030    -1.579642      27.06
 O      -5.281383    -0.095434     0.358513     120.97
 H      -4.795339     0.294793     1.145832      26.32
 C      -3.210428    -1.151826    -0.751079      72.09
 H      -2.497080    -1.199661    -1.559687      24.06
 C      -3.827352    -2.587727    -0.486749     100.63
 O      -4.733710    -2.949312    -1.569778     229.47
 H      -4.107251    -3.237095    -2.140363      32.04
 H      -4.562629    -2.550371     0.339688      25.34
 H      -2.867729    -3.289210    -0.173232      24.84
 C       1.120644    -1.424611    -0.906248      35.85
 H       1.633818    -1.898084    -1.817663      23.32
 C       1.231297     0.028795     1.232016     107.69
 H       2.083471     0.015009     2.010202      20.85
 C      -0.135847     0.107779     1.268856       7.63
 O      -0.888531     0.487165     2.389686     207.05
 C      -0.175467     0.698518     3.565129     124.48
 H       0.506313     1.485739     3.387910      28.34
 H      -0.604282     1.507368     4.251526      26.13
 H       0.685910    -0.145082     3.823991      25.20
 C      -0.986117    -0.748795     0.216294       1.27
 O      -2.323414    -0.872696     0.444394     169.34
 C      -0.311409    -1.349807    -0.800754      75.75
 H      -0.909454    -1.917726    -1.463956      24.18
 C       1.939371    -0.696125     0.005697      14.39
 C       3.381071    -0.340376    -0.459450      70.95
 H       3.463291    -0.468602    -1.665345      25.12
 O       3.497998     1.192809    -0.301286     144.33
 H       3.878444     1.449346     0.558738      26.41
 C       4.519257    -1.015843     0.276150     106.92
 H       4.628121    -0.651371     1.219127      29.75
 O       4.269050    -2.535519     0.372640     204.45
 H       4.344158    -3.108175    -0.490131      27.71
 C       5.842306    -0.713762    -0.310841      84.05
 O       6.362574     0.808118    -0.256595     158.65
 H       6.658257     0.895225     0.656206      27.81
 H       5.909414    -1.040289    -1.465152      28.54
 H       6.765058    -1.290189     0.265512      28.56
55
name= lig-ACN-Water-frame_728
 C      -3.827806     1.478128    -2.797570      53.18
 H      -3.495488     0.485419    -3.477136      20.48
 C      -3.987860     2.553302    -0.474794      64.56
 H      -4.306308     2.497404     0.620128      24.84
 C      -3.730548     3.807587    -1.071366      14.30
 O      -3.631108     4.970649    -0.488834     182.82
 C      -3.118390     4.886798     1.007126      86.28
 H      -4.006264     5.479810     1.511185      23.09
 H      -2.020274     5.352569     0.981319      24.53
 H      -3.107055     3.769434     1.429281      23.22
 C      -3.751492     3.941691    -2.428706      16.42
 O      -3.375628     5.087315    -3.149917     103.23
 H      -3.311392     5.820896    -2.512269      26.94
 C      -3.712336     2.807863    -3.269778       4.39
 H      -3.512404     3.123279    -4.408902      19.89
 C      -4.005032     1.417310    -1.405659      -1.99
 C      -4.403094    -0.062079    -0.852891      80.47
 H      -4.980893    -0.359968    -1.639052      28.34
 O      -5.311176    -0.009977     0.277749     167.21
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 H      -4.666737    -0.026371     1.066096      28.76
 C      -3.179939    -1.173345    -0.770658      74.70
 H      -2.747902    -1.058028    -1.832324      24.21
 C      -3.754667    -2.542441    -0.485287     108.22
 O      -4.672465    -2.949062    -1.604833     230.60
 H      -4.352749    -3.059741    -2.507837      28.18
 H      -4.250659    -2.410620     0.519475      26.12
 H      -2.935673    -3.422813    -0.351605      25.00
 C       1.061861    -1.344867    -0.888676      30.41
 H       1.601292    -1.769941    -1.819695      19.31
 C       1.358478     0.015025     1.270732      90.71
 H       1.746805     0.548113     2.158941      12.63
 C      -0.093398    -0.051544     1.358737      31.39
 O      -0.914743     0.458435     2.387198     175.41
 C      -0.127978     0.761709     3.641556      98.03
 H       0.596214     1.391534     3.387856      28.66
 H      -1.114787     0.852490     4.388466      22.56
 H       0.259570    -0.294532     4.232791      24.98
 C      -0.944654    -0.733947     0.298307       9.40
 O      -2.387112    -0.886573     0.474186     134.81
 C      -0.380001    -1.422521    -0.861655      65.03
 H      -0.795451    -1.836887    -1.816971      19.49
 C       1.868866    -0.591008     0.024473      21.11
 C       3.266826    -0.282266    -0.402304      81.62
 H       3.440246    -0.570960    -1.592008      20.31
 O       3.527210     1.097010    -0.345149     241.77
 H       3.447205     1.307991     0.599845      25.44
 C       4.455197    -1.025231     0.259517      86.76
 H       4.335837    -0.825132     1.281091      28.74
 O       4.243150    -2.554703     0.374247     269.57
 H       4.281058    -2.732531    -0.594557      29.32
 C       6.004372    -0.621673    -0.373595      83.02
 O       6.339722     0.688477    -0.261136     273.90
 H       6.568922     1.156696     0.645257      25.73
 H       6.153839    -0.921723    -1.530596      26.90
 H       6.574686    -1.437111     0.328036      27.28
55
name= lig-ACN-Water-frame_729
 C      -3.917134     1.620089    -2.772579      40.79
 H      -3.800118     0.657778    -3.603443      22.18
 C      -4.012946     2.447326    -0.524723      84.34
 H      -4.274366     2.305722     0.483222      27.89
 C      -3.813473     3.775437    -1.040817      -9.16
 O      -3.550212     4.999163    -0.351881     231.04
 C      -3.188997     4.940705     0.889449     111.37
 H      -3.668229     5.616291     1.748404      24.20
 H      -2.051844     5.356516     1.077590      26.18
 H      -3.207070     3.888907     1.293993      25.29
 C      -3.672653     3.950164    -2.470996       0.05
 O      -3.394869     5.099361    -3.213906     119.16
 H      -3.193085     5.904933    -2.695059      23.48
 C      -3.655556     2.841609    -3.290946      43.52
 H      -3.369982     2.911510    -4.481734      22.29
 C      -4.065303     1.347837    -1.358638      10.10
 C      -4.350363    -0.028491    -0.872199     100.02
 H      -4.909755    -0.594119    -1.565535      28.82
 O      -5.276220     0.040614     0.241733     149.10
 H      -4.883134     0.001929     1.111616      28.90
 C      -3.258456    -1.040619    -0.683248      84.23
 H      -2.477468    -0.983437    -1.593665      23.78
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 C      -3.756968    -2.547520    -0.572347     105.38
 O      -4.699149    -2.935672    -1.517941     220.43
 H      -3.883462    -2.969999    -2.262190      24.46
 H      -4.325721    -2.774746     0.328678      24.83
 H      -2.732605    -3.249436    -0.666449      23.79
 C       1.029842    -1.201171    -0.913035      70.55
 H       1.523623    -1.638106    -1.846492      21.24
 C       1.226736    -0.059956     1.213353      67.49
 H       1.850705     0.670945     1.552997      15.29
 C      -0.187971    -0.294567     1.347248      39.01
 O      -0.834626     0.408497     2.398188     160.36
 C      -0.224238     0.731595     3.704816      93.43
 H       0.475851     1.536355     3.911155      27.04
 H      -1.063164     1.348835     4.457821      23.19
 H       0.346696    -0.335248     3.913625      26.44
 C      -0.950742    -0.810120     0.312551      28.48
 O      -2.358236    -0.810669     0.460694     209.58
 C      -0.334671    -1.373646    -0.760634      46.37
 H      -1.112589    -1.939343    -1.415966      17.68
 C       1.818094    -0.521705     0.083864      49.28
 C       3.245495    -0.326231    -0.427735      67.15
 H       3.026342    -0.593127    -1.605893      21.11
 O       3.562738     1.103220    -0.356415     213.14
 H       3.633017     1.408278     0.622623      25.76
 C       4.474185    -1.102229     0.326621      91.95
 H       4.611452    -0.683782     1.295279      27.47
 O       4.258615    -2.464968     0.264400     294.69
 H       4.120475    -2.841638    -0.578789      31.84
 C       5.967455    -0.749440    -0.268839      86.56
 O       6.358979     0.691445    -0.293034     228.15
 H       6.420867     0.961547     0.707612      27.39
 H       5.911157    -1.023048    -1.415508      28.78
 H       6.951082    -1.304867     0.180347      28.76
55
name= lig-ACN-Water-frame_730
 C      -3.950699     1.568298    -2.770921      48.62
 H      -4.464034     0.665079    -3.467537      21.62
 C      -4.061422     2.459468    -0.515482      55.51
 H      -3.920896     2.293716     0.453437      22.09
 C      -3.833331     3.814112    -1.123485     -26.55
 O      -3.596038     5.013820    -0.401713     214.51
 C      -3.092120     4.963681     1.145661      72.39
 H      -3.927494     5.765870     1.457405      21.55
 H      -1.988550     5.314142     0.976570      24.58
 H      -3.195848     4.012429     1.623634      26.15
 C      -3.530371     3.972644    -2.558709      -0.45
 O      -3.405162     5.197235    -3.224469     181.30
 H      -3.556161     5.974156    -2.567011      21.26
 C      -3.626996     2.824522    -3.345432      42.85
 H      -3.442245     2.975360    -4.550660      22.07
 C      -4.105521     1.327810    -1.407080      15.82
 C      -4.412809    -0.054011    -0.891599      80.30
 H      -4.926649    -0.521446    -1.733030      25.91
 O      -5.302848     0.045532     0.282762     167.57
 H      -4.635865     0.349837     0.934518      29.42
 C      -3.196504    -0.970671    -0.593134      73.53
 H      -2.684391    -0.903231    -1.709104      22.27
 C      -3.712671    -2.547825    -0.517041      99.00
 O      -4.725184    -2.917661    -1.541548     201.53
 H      -4.534863    -3.378213    -2.467991      26.18
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 H      -3.940660    -2.727419     0.584266      26.40
 H      -2.686594    -3.081032    -0.708837      24.48
 C       1.025979    -1.175407    -1.036565      28.95
 H       1.498294    -1.516779    -1.995919      20.83
 C       1.083763    -0.080536     1.168085      78.46
 H       1.360548     0.404642     2.012813      22.55
 C      -0.222559    -0.283836     1.456819      26.40
 O      -0.824952     0.398227     2.435847     219.95
 C      -0.261749     0.667449     3.708516     105.65
 H       0.329071     1.431134     3.349863      24.01
 H      -1.406467     0.968105     4.286789      21.67
 H       0.236048    -0.095869     4.473206      25.42
 C      -1.054149    -0.909047     0.420507      21.78
 O      -2.386298    -0.687496     0.518441     177.44
 C      -0.357485    -1.366498    -0.730184      57.96
 H      -0.692640    -2.104905    -1.596179      20.14
 C       1.882721    -0.610938    -0.020132      29.28
 C       3.346062    -0.300632    -0.373269      72.97
 H       3.740497    -0.531745    -1.497569      22.17
 O       3.616977     1.176064    -0.348480     192.49
 H       4.080458     1.276107     0.544893      25.25
 C       4.518270    -1.019637     0.327140     113.96
 H       4.331024    -1.016175     1.373208      27.08
 O       4.268858    -2.496195     0.190000     252.59
 H       4.289398    -2.603114    -0.814604      28.17
 C       5.864910    -0.836806    -0.258765      94.46
 O       6.350289     0.672797    -0.294686     171.49
 H       6.729311     0.988497     0.546302      27.29
 H       5.904423    -1.218514    -1.340365      30.26
 H       6.527295    -1.554530     0.431854      28.56
55
name= lig-ACN-Water-frame_731
55
name= lig-ACN-Water-frame_732
 C      -4.025599     1.548647    -2.845300      57.01
 H      -3.902017     0.598065    -3.446776      23.65
 C      -3.931705     2.562552    -0.700793      34.89
 H      -4.362296     2.452694     0.273265      25.70
 C      -3.516555     3.870448    -1.163918     -28.34
 O      -3.666430     5.007871    -0.220797     203.85
 C      -3.125810     5.029031     1.096866     100.82
 H      -3.772635     6.020844     1.666882      21.27
 H      -2.082844     5.127825     0.934421      27.22
 H      -3.372538     4.134861     1.630900      26.73
 C      -3.548614     4.005397    -2.640412       3.67
 O      -3.377771     5.204346    -3.166898      69.84
 H      -3.346360     5.974062    -2.474399      22.59
 C      -3.725047     2.809542    -3.431755      62.81
 H      -3.549298     2.920512    -4.527480      22.57
 C      -4.202435     1.389515    -1.445026      22.01
 C      -4.536077     0.016168    -0.798386      77.68
 H      -5.264184    -0.376770    -1.646061      23.40
 O      -5.344153    -0.034597     0.437151     165.50
 H      -4.915865     0.548850     1.081275      29.18
 C      -3.295549    -0.963722    -0.667944      55.39
 H      -2.781413    -0.803847    -1.800335      25.24
 C      -3.706101    -2.530205    -0.546408     127.27
 O      -4.673892    -2.853602    -1.469616     264.88
 H      -4.597665    -2.898360    -2.387169      29.54
 H      -3.948430    -2.601566     0.606188      25.66
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 H      -2.752920    -2.982397    -0.523974      27.60
 C       0.985133    -1.232124    -1.014494      42.36
 H       1.473778    -1.503178    -1.954740      21.62
 C       1.306356    -0.224174     1.233563      84.28
 H       1.829110     0.360313     2.000282      20.83
 C      -0.066884    -0.192822     1.387612      -4.82
 O      -0.955907     0.246490     2.464272     127.75
 C      -0.224037     0.672868     3.777917      83.26
 H       0.474636     1.425738     3.258732      23.97
 H      -1.228659     1.078160     4.439285      23.45
 H       0.150540    -0.240936     4.306701      26.31
 C      -1.081575    -0.835824     0.335587       1.80
 O      -2.470996    -0.641621     0.523551     109.08
 C      -0.471028    -1.421967    -0.759163      72.45
 H      -0.847938    -1.875502    -1.716364      23.44
 C       1.834760    -0.538632    -0.189454      32.22
 C       3.281662    -0.197853    -0.399086      71.03
 H       3.675425    -0.205668    -1.466369      22.14
 O       3.786305     1.267179    -0.211189     200.52
 H       3.660198     1.390375     0.756377      25.73
 C       4.512283    -1.143516     0.319077      85.86
 H       4.186208    -1.225144     1.417934      25.86
 O       4.237893    -2.512350     0.090225     297.21
 H       4.446042    -2.589656    -0.885005      29.13
 C       5.921349    -0.861961    -0.159229     100.62
 O       6.400331     0.551801    -0.257331     265.39
 H       6.580915     1.032507     0.645397      27.09
 H       5.862341    -1.222992    -1.179269      31.18
 H       6.709162    -1.527059     0.356687      28.25
55
name= lig-ACN-Water-frame_733
 C      -3.972412     1.576318    -2.853090      33.94
 H      -4.212350     0.838257    -3.600405      20.44
 C      -3.942833     2.536283    -0.655205      57.78
 H      -4.009647     2.568657     0.477757      23.52
 C      -3.516728     3.802596    -1.107281      -4.80
 O      -3.714362     5.036627    -0.312181     227.93
 C      -3.115314     4.978776     1.004392     116.41
 H      -3.510443     6.093177     1.564495      22.26
 H      -2.091876     5.105776     1.153105      28.81
 H      -3.412264     4.131153     1.686432      25.44
 C      -3.552739     3.992277    -2.495576       0.82
 O      -3.330284     5.195194    -3.242636     174.84
 H      -3.636197     5.948774    -2.725907      21.90
 C      -3.795008     2.874728    -3.413171      36.72
 H      -3.589426     2.965783    -4.422119      28.31
 C      -4.175481     1.418137    -1.454163      52.49
 C      -4.570403     0.058986    -0.756347      88.60
 H      -5.180226    -0.698482    -1.478650      25.16
 O      -5.363851    -0.024626     0.498105     182.27
 H      -4.760969     0.100535     1.260702      26.03
 C      -3.384637    -0.894321    -0.648882      74.81
 H      -2.686336    -0.831060    -1.671441      25.06
 C      -3.701845    -2.369108    -0.494117     118.11
 O      -4.685279    -2.920001    -1.488662     171.64
 H      -4.181827    -2.434704    -2.317547      27.43
 H      -4.366199    -2.748283     0.352514      24.32
 H      -2.882458    -2.935324    -0.741201      27.38
 C       0.949084    -1.229539    -0.994461      59.34
 H       1.224301    -1.764941    -1.918827      21.99
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 C       1.243643    -0.191068     1.192755      59.12
 H       1.893412     0.215030     2.067965      19.27
 C      -0.216874    -0.245134     1.334462      32.26
 O      -0.759858     0.145529     2.462267     225.76
 C      -0.217720     0.607176     3.639490     108.77
 H       0.627019     1.594682     3.655552      23.18
 H      -1.098453     1.285586     4.222814      23.60
 H       0.274280    -0.157807     4.221774      27.26
 C      -0.971528    -0.610706     0.275038      28.32
 O      -2.369991    -0.710149     0.388632     156.32
 C      -0.409869    -1.357905    -0.798390      57.50
 H      -1.096510    -2.035492    -1.290528      23.43
 C       1.815199    -0.484897    -0.024885      19.70
 C       3.381426    -0.210026    -0.484655      71.71
 H       3.344221    -0.442217    -1.571994      24.46
 O       3.726220     1.240660    -0.085290     202.32
 H       3.885418     1.361278     0.935924      21.67
 C       4.399547    -1.133783     0.280113      78.67
 H       4.541213    -0.750421     1.426067      23.85
 O       4.201443    -2.567730     0.034915     274.23
 H       4.179759    -2.845980    -0.875776      30.29
 C       5.977911    -0.903886    -0.172997      94.35
 O       6.468109     0.533822    -0.233038     249.92
 H       6.562472     0.894351     0.753318      27.02
 H       6.193998    -1.172259    -1.152900      31.65
 H       6.511061    -1.617697     0.530227      31.00
55
name= lig-ACN-Water-frame_734
 C      -4.051851     1.592674    -2.883357      52.39
 H      -4.309982     0.802096    -3.502386      24.89
 C      -3.923626     2.548866    -0.482619      38.47
 H      -3.908980     2.234719     0.678886      19.89
 C      -3.711979     3.832351    -1.093631       0.31
 O      -3.704155     4.978120    -0.484658     203.23
 C      -3.064340     4.985874     1.030019      80.59
 H      -3.526804     6.069906     1.570961      22.64
 H      -2.084270     4.813615     0.821559      28.87
 H      -3.668488     4.097004     1.510463      22.52
 C      -3.520529     4.007745    -2.541981      19.98
 O      -3.314109     5.179894    -3.259238     166.81
 H      -3.309618     5.998605    -2.761919      24.39
 C      -3.748135     2.914150    -3.285237      63.73
 H      -3.935448     3.138687    -4.246285      25.88
 C      -4.148093     1.442043    -1.374891     -43.76
 C      -4.569295     0.022396    -0.723208      68.33
 H      -5.409947    -0.329634    -1.531373      23.59
 O      -5.354371     0.050303     0.523146     189.58
 H      -4.754052    -0.211464     1.296238      25.59
 C      -3.293763    -0.915627    -0.696597      69.99
 H      -2.898925    -0.721711    -1.817788      24.33
 C      -3.774636    -2.381993    -0.481181     124.19
 O      -4.682402    -2.899225    -1.565712     188.58
 H      -4.207648    -3.049753    -2.523760      24.26
 H      -4.005811    -2.308478     0.628328      25.71
 H      -2.914673    -2.944273    -0.290890      26.70
 C       1.078272    -1.196916    -0.990249      53.39
 H       1.720111    -1.735078    -1.732169      21.66
 C       1.162892    -0.098114     1.128916      82.22
 H       1.851829     0.175471     2.066939      20.00
 C      -0.133721    -0.221630     1.287372      16.93
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 O      -0.780551     0.044996     2.482538     186.97
 C      -0.088024     0.666974     3.633948      93.71
 H       0.803221     1.475966     3.335460      21.82
 H      -1.057834     1.064996     4.256990      23.67
 H       0.198354    -0.261648     4.206574      24.96
 C      -1.008082    -0.553363     0.119407      20.71
 O      -2.362515    -0.654321     0.409542     170.70
 C      -0.343770    -1.258468    -0.836769      67.47
 H      -0.878209    -1.899374    -1.471600      24.88
 C       1.862650    -0.590669    -0.062887      21.83
 C       3.355278    -0.161571    -0.385729      97.96
 H       3.455640    -0.049282    -1.447458      25.17
 O       3.617968     1.130131    -0.073146     242.12
 H       3.889660     1.252963     0.943145      22.45
 C       4.457327    -1.108036     0.122967      88.89
 H       4.182586    -1.051200     1.339638      23.86
 O       4.128498    -2.602192     0.036245     282.31
 H       4.217173    -2.717101    -0.959825      28.13
 C       5.982356    -0.846360    -0.205303     118.37
 O       6.509640     0.423184    -0.211635     300.01
 H       6.955990     0.700289     0.640038      27.32
 H       6.138824    -1.418494    -1.061049      32.47
 H       6.569915    -1.325391     0.574574      28.99
55
name= lig-ACN-Water-frame_735
 C      -4.171492     1.616959    -2.641310      73.07
 H      -4.310854     0.831721    -3.323254      26.59
 C      -3.902410     2.524964    -0.510364      30.19
 H      -4.140650     2.566098     0.694666      18.51
 C      -3.839173     3.825958    -1.137365       8.58
 O      -3.634864     5.091121    -0.396807     230.11
 C      -3.143705     4.939175     0.855966     106.41
 H      -3.108653     6.092154     1.323698      23.89
 H      -2.076729     4.726891     0.951437      29.70
 H      -3.582391     4.159112     1.693659      23.36
 C      -3.539344     4.010801    -2.499213     -21.99
 O      -3.291938     5.188555    -3.219714     154.02
 H      -3.236158     5.920409    -2.504188      18.49
 C      -3.773539     2.791300    -3.383989      19.68
 H      -3.740833     2.915422    -4.429210      21.69
 C      -4.150683     1.418665    -1.284002      46.27
 C      -4.501282     0.081451    -0.746022      72.20
 H      -5.169531    -0.555393    -1.563134      24.47
 O      -5.306904     0.118941     0.515670     165.71
 H      -4.683716     0.090531     1.287987      25.72
 C      -3.301670    -0.963030    -0.780423      77.65
 H      -2.591957    -0.892542    -1.681465      27.83
 C      -3.766781    -2.451434    -0.511385     121.14
 O      -4.641068    -2.855510    -1.569796     215.38
 H      -4.105714    -3.410476    -2.045611      31.37
 H      -4.616405    -2.446682     0.133364      27.81
 H      -3.045130    -3.180781    -0.404195      29.02
 C       1.187371    -1.256585    -1.050924      35.86
 H       1.539050    -1.631208    -2.065903      19.57
 C       1.327231    -0.052881     1.062461      55.75
 H       1.876378     0.471671     1.964862      16.95
 C      -0.194020    -0.111074     1.229529       1.83
 O      -0.878665     0.012488     2.476630     146.41
 C      -0.021633     0.601324     3.634525      93.71
 H       0.720838     1.409448     3.027608      23.73
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 H      -0.638246     1.412108     4.293824      24.73
 H       0.556970    -0.189071     4.124775      26.76
 C      -0.996269    -0.603200     0.173108      -6.77
 O      -2.427574    -0.529508     0.401824     114.60
 C      -0.238086    -1.226424    -1.045931      52.02
 H      -0.666596    -1.467480    -1.959492      24.23
 C       1.935945    -0.579480    -0.045435      30.98
 C       3.303602    -0.234678    -0.446807      89.05
 H       3.336319    -0.375008    -1.477748      24.04
 O       3.550436     1.190954    -0.051752     231.02
 H       3.572277     1.337901     1.001577      20.45
 C       4.461648    -1.188829     0.182348      69.65
 H       4.528062    -0.991861     1.438110      23.73
 O       4.090243    -2.531237    -0.038114     275.50
 H       4.315920    -3.016368    -0.958060      27.32
 C       5.974166    -0.987192    -0.178929     105.52
 O       6.565831     0.425690    -0.270122     299.21
 H       6.795940     0.723465     0.615613      30.01
 H       6.188857    -1.232951    -1.172609      32.63
 H       6.427526    -1.696280     0.483604      31.95
55
name= lig-ACN-Water-frame_736
 C      -4.202683     1.592399    -2.681382      30.04
 H      -4.498946     0.620049    -3.129757      28.23
 C      -3.979094     2.690402    -0.502039      48.39
 H      -3.994779     2.645573     0.703747      22.95
 C      -3.769019     3.913965    -1.133756      -2.11
 O      -3.665880     5.101494    -0.453594     195.32
 C      -3.049551     4.961964     0.923913      98.51
 H      -3.049975     6.024859     1.375214      23.91
 H      -2.139954     4.356832     0.778907      27.13
 H      -3.985587     4.384221     1.515727      22.40
 C      -3.661460     3.906747    -2.613254       0.86
 O      -3.258856     5.150936    -3.107837      81.46
 H      -3.545380     6.077978    -2.681935      24.34
 C      -3.838321     2.750229    -3.314846     108.95
 H      -3.454878     2.493636    -4.322027      22.17
 C      -4.167580     1.444431    -1.204440     -82.48
 C      -4.455845    -0.001488    -0.752460      54.11
 H      -5.341446    -0.372280    -1.483908      19.38
 O      -5.195947     0.138067     0.470513     179.82
 H      -4.699751     0.657315     1.113351      27.27
 C      -3.268229    -0.985493    -0.673925      97.70
 H      -2.912842    -0.945969    -1.737670      27.92
 C      -3.817211    -2.430058    -0.489016     140.63
 O      -4.611265    -2.890667    -1.665606     153.41
 H      -4.117109    -3.346818    -2.403468      24.73
 H      -4.075152    -2.471262     0.559386      27.09
 H      -2.911112    -2.975462    -0.343781      27.18
 C       1.142853    -1.253380    -1.121113      38.23
 H       1.750170    -1.565210    -2.032859      18.75
 C       1.238484    -0.026260     1.081856      64.30
 H       1.961664     0.598811     1.625122      15.77
 C      -0.145621    -0.117714     1.214904       3.49
 O      -0.877783     0.079732     2.495454     184.13
 C      -0.013028     0.568047     3.446815     108.11
 H       0.772023     1.348215     3.108035      24.75
 H      -0.652977     1.190761     4.216367      25.34
 H       0.610447    -0.294180     3.956031      25.22
 C      -0.889400    -0.728875     0.117859       6.76
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 O      -2.390541    -0.459791     0.295647     134.71
 C      -0.272166    -1.101957    -1.061762      68.42
 H      -0.966747    -1.409132    -1.825434      23.56
 C       1.913020    -0.617084    -0.095523      17.22
 C       3.474520    -0.237765    -0.434432      82.23
 H       3.620934    -0.239296    -1.455702      19.80
 O       3.495620     1.243223    -0.134830     245.03
 H       3.941015     1.331576     0.805762      22.46
 C       4.451072    -1.164352     0.262197      85.19
 H       4.298542    -1.005113     1.503367      23.34
 O       4.062021    -2.549033    -0.085172     318.54
 H       4.344160    -2.449693    -1.092296      24.34
 C       6.012105    -1.041299    -0.261169     110.86
 O       6.570663     0.339398    -0.305919     318.82
 H       6.597446     0.763068     0.571035      33.34
 H       5.952750    -1.480791    -1.251467      34.13
 H       6.699011    -1.580135     0.268815      30.02
55
name= lig-ACN-Water-frame_737
 C      -4.193655     1.471420    -2.633539      68.47
 H      -4.176060     0.611736    -3.404745      22.45
 C      -4.066363     2.705277    -0.465552      63.59
 H      -3.813349     2.620366     0.638834      17.36
 C      -3.743341     3.894181    -1.174157      -3.94
 O      -3.660182     5.136721    -0.532080     173.92
 C      -3.062982     4.987053     0.983517      72.70
 H      -2.587765     5.854384     1.260336      25.40
 H      -2.175421     4.166795     0.976206      24.94
 H      -3.877605     4.550774     1.789391      23.87
 C      -3.754195     3.985835    -2.548118      -4.71
 O      -3.220544     5.088596    -3.135883     139.87
 H      -3.500390     5.820849    -2.487961      22.56
 C      -3.857762     2.711960    -3.315648       5.41
 H      -3.724856     2.981788    -4.475069      15.98
 C      -4.201808     1.533029    -1.303724      22.04
 C      -4.479470     0.083195    -0.696790      77.58
 H      -5.098909    -0.540777    -1.500835      23.76
 O      -5.145259     0.100552     0.525127     217.30
 H      -4.598116     0.689368     1.140604      25.33
 C      -3.315194    -0.929746    -0.708753      85.12
 H      -2.865257    -0.948011    -1.699686      26.83
 C      -3.696507    -2.439586    -0.463067     107.11
 O      -4.601761    -2.924517    -1.676150     124.93
 H      -3.845061    -2.751198    -2.452275      25.97
 H      -4.423811    -2.715842     0.216605      27.00
 H      -2.826035    -3.061655    -0.669821      25.26
 C       1.095703    -1.137514    -1.164744      45.10
 H       1.508227    -1.709182    -2.048148      20.83
 C       1.226949    -0.048140     0.979611      87.81
 H       1.656638     0.446695     1.769866      18.73
 C      -0.149187    -0.284639     1.249425      23.99
 O      -0.831425     0.176970     2.290752     192.20
 C       0.027361     0.579037     3.436584     108.05
 H       0.658448     1.587815     3.193287      22.45
 H      -0.682617     0.832166     4.262698      25.17
 H       0.606105    -0.367858     3.704162      26.34
 C      -0.954940    -0.673771     0.175445      23.96
 O      -2.209280    -0.475928     0.191858     162.25
 C      -0.329521    -1.096961    -1.067370      61.93
 H      -0.885523    -1.645569    -1.918820      21.89
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 C       1.923192    -0.593803    -0.183053      42.27
 C       3.444546    -0.143088    -0.387953      82.33
 H       3.705431    -0.365113    -1.370553      21.81
 O       3.532289     1.234495    -0.230467     295.31
 H       3.889821     1.471644     0.650998      25.82
 C       4.555239    -1.152784     0.300920      80.97
 H       4.421761    -1.276862     1.529285      22.81
 O       4.058791    -2.521873    -0.105216     349.69
 H       4.166390    -2.904914    -1.007672      27.10
 C       5.979689    -1.023922    -0.272674     124.85
 O       6.533240     0.243265    -0.388677     306.56
 H       6.949105     0.439837     0.554484      29.44
 H       5.971481    -1.312019    -1.362661      32.37
 H       6.517036    -1.709631     0.244057      30.26
55
name= lig-ACN-Water-frame_738
 C      -4.061316     1.576024    -2.774016      20.79
 H      -4.102656     0.527086    -3.236599      22.09
 C      -4.075045     2.606673    -0.532117      49.58
 H      -4.198167     2.528174     0.517855      21.98
 C      -3.865139     3.899226    -1.079680      -4.59
 O      -3.557027     5.132177    -0.410090     234.85
 C      -3.089746     5.003857     0.887557     110.28
 H      -2.622463     5.830055     1.037211      26.34
 H      -2.382439     3.990497     1.012811      25.45
 H      -3.959071     5.024963     1.716740      21.82
 C      -3.716256     3.895894    -2.528949       6.04
 O      -3.232999     5.070240    -3.233153     170.80
 H      -3.039548     5.842880    -2.729883      24.11
 C      -3.921355     2.814653    -3.330821      87.32
 H      -4.058940     2.814835    -4.545317      26.14
 C      -4.268713     1.444001    -1.274432      19.67
 C      -4.474474     0.143101    -0.674358      80.71
 H      -5.370335    -0.257131    -1.265574      24.42
 O      -5.172987     0.062306     0.662739     191.97
 H      -4.527649     0.131651     1.470364      23.59
 C      -3.223830    -0.892564    -0.794702      82.26
 H      -2.867812    -0.796417    -1.802470      27.12
 C      -3.681995    -2.479180    -0.616920     120.22
 O      -4.485524    -2.881044    -1.651144     240.76
 H      -4.278981    -2.608274    -2.591524      26.07
 H      -4.041214    -2.551442     0.345929      27.01
 H      -2.691324    -2.970616    -0.373562      25.96
 C       1.082090    -1.064338    -1.250713      43.64
 H       1.468155    -1.460522    -2.207819      23.08
 C       1.290688    -0.148184     0.948909      62.50
 H       1.939733     0.208437     1.638745      20.60
 C      -0.092527    -0.393076     1.124776       3.91
 O      -0.796182     0.331253     2.206163     139.64
 C      -0.015063     0.555583     3.459701     114.91
 H       0.511182     1.599753     3.303591      25.28
 H      -0.682418     0.741373     4.248945      28.02
 H       0.938148    -0.101830     3.626550      25.14
 C      -0.885137    -0.708948    -0.001391       7.24
 O      -2.344704    -0.455795     0.216196     127.78
 C      -0.283768    -1.219450    -1.046014      73.36
 H      -1.001519    -1.618813    -1.923342      22.29
 C       1.935677    -0.454212    -0.211617      18.66
 C       3.395688    -0.256252    -0.420556      93.12
 H       3.434032    -0.392206    -1.472609      21.64
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 O       3.634016     1.300353    -0.275700     222.07
 H       3.652741     1.411456     0.688776      25.72
 C       4.474895    -1.194523     0.243011     100.72
 H       4.743871    -0.941089     1.382824      23.30
 O       4.060083    -2.507944    -0.045103     321.24
 H       4.408847    -2.524340    -0.928389      28.06
 C       5.922714    -1.119260    -0.331583     112.37
 O       6.572589     0.267199    -0.397758     270.28
 H       7.046779     0.515752     0.500833      28.70
 H       5.860970    -1.488413    -1.427037      31.26
 H       6.521810    -1.744210     0.135876      30.57
55
name= lig-ACN-Water-frame_739
 C      -4.031412     1.565008    -2.735277      44.46
 H      -4.234461     0.843250    -3.541092      20.69
 C      -4.147909     2.597675    -0.494454      64.09
 H      -4.484447     2.468825     0.434553      22.56
 C      -3.906793     3.917119    -1.101453       9.72
 O      -3.510034     5.015290    -0.448810     226.38
 C      -3.107445     5.034389     0.963426      94.75
 H      -2.418861     5.758871     1.235099      25.70
 H      -2.549476     3.944842     1.310489      25.16
 H      -4.036256     5.075898     1.606375      22.90
 C      -3.620670     4.002027    -2.531913      -5.32
 O      -3.272801     5.031864    -3.308240     192.57
 H      -3.487338     5.863977    -2.788093      22.28
 C      -3.990620     2.854120    -3.351675      20.87
 H      -3.727764     3.029465    -4.545875      24.06
 C      -4.193470     1.475736    -1.372332      24.40
 C      -4.592715    -0.040464    -0.609977      88.02
 H      -5.300285    -0.563818    -1.263740      25.37
 O      -5.173609     0.023685     0.718884     253.78
 H      -4.464029     0.279204     1.415463      22.90
 C      -3.297284    -0.866063    -0.872245      88.53
 H      -2.832002    -0.600328    -1.745907      28.08
 C      -3.504749    -2.276667    -0.689091     115.22
 O      -4.478347    -2.897599    -1.678642     206.82
 H      -4.022658    -2.728237    -2.445057      32.56
 H      -4.086847    -2.471852     0.140669      26.69
 H      -2.640070    -2.912716    -1.025919      23.92
 C       1.184646    -1.032740    -1.368769      30.21
 H       1.790723    -1.173591    -2.239531      19.70
 C       1.341285    -0.265543     1.041596      67.79
 H       1.764256     0.176421     1.911475      19.38
 C      -0.075701    -0.195805     1.108732      -2.74
 O      -0.723437     0.377658     2.172360     193.48
 C      -0.058058     0.611692     3.379826     118.72
 H       0.273220     1.755567     3.644163      23.33
 H      -0.731392     0.299887     4.118256      26.68
 H       0.669972    -0.269340     3.487357      24.26
 C      -0.991215    -0.721967     0.046461     -24.78
 O      -2.361601    -0.477882     0.245252     101.61
 C      -0.255385    -1.357062    -1.193789      40.00
 H      -0.820215    -1.849057    -2.176856      19.44
 C       1.897576    -0.491925    -0.323033      25.52
 C       3.418484    -0.190327    -0.590236      80.18
 H       3.811209    -0.272045    -1.609663      21.80
 O       3.734147     1.249854    -0.301438     224.01
 H       3.956466     1.438826     0.693597      24.91
 C       4.415685    -1.113391     0.190625      75.29
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 H       4.093656    -1.024900     1.288136      24.70
 O       4.068745    -2.560531     0.024634     307.09
 H       3.995046    -2.871177    -0.918469      28.95
 C       5.964982    -1.036275    -0.422853     113.95
 O       6.599553     0.223049    -0.381543     301.70
 H       6.657328     0.392094     0.556811      33.47
 H       5.990132    -1.325883    -1.544940      30.56
 H       6.431885    -1.721658     0.094675      31.17
55
name= lig-ACN-Water-frame_740
 C      -4.124592     1.565783    -2.778525      69.45
 H      -4.109662     0.669555    -3.301519      25.31
 C      -4.274032     2.646035    -0.558658      82.14
 H      -4.307119     2.704299     0.434012      26.01
 C      -3.786089     3.811477    -1.179527     -13.40
 O      -3.455667     5.025100    -0.466248     125.08
 C      -3.175080     4.961485     1.108691      85.05
 H      -2.393242     5.780556     1.049693      23.94
 H      -2.715479     3.842057     1.382675      23.85
 H      -4.007269     5.266794     1.729947      24.41
 C      -3.726289     3.958413    -2.553777      27.98
 O      -3.305383     5.147135    -3.319173     111.19
 H      -3.578806     6.114347    -2.948434      22.93
 C      -3.885809     2.833606    -3.308008      70.72
 H      -3.769858     2.965218    -4.479306      20.13
 C      -4.249727     1.390041    -1.292938     -55.47
 C      -4.658828    -0.019529    -0.688959      94.84
 H      -5.392699    -0.589318    -1.192715      24.71
 O      -5.166060    -0.026185     0.644799     242.27
 H      -4.595377     0.284225     1.370565      24.74
 C      -3.309942    -0.736792    -0.834255      85.66
 H      -3.006843    -0.453561    -1.731313      30.36
 C      -3.401385    -2.333656    -0.780473     107.42
 O      -4.476119    -2.878841    -1.762617     149.95
 H      -4.121361    -3.338118    -2.649365      24.14
 H      -3.581378    -2.560237     0.258729      26.55
 H      -2.318212    -2.704709    -0.731706      24.95
 C       1.120810    -1.060954    -1.410566      40.18
 H       1.414401    -1.389813    -2.368979      20.51
 C       1.322254    -0.313567     0.931766      76.16
 H       2.137443     0.024769     1.626175      18.09
 C      -0.095845    -0.081709     0.971163       8.77
 O      -0.761148     0.432415     2.109267     181.44
 C      -0.114904     0.563836     3.433951     112.38
 H       0.276221     1.699262     3.476617      23.60
 H      -0.840607     0.447180     4.091236      27.25
 H       0.934046     0.062580     3.568741      23.69
 C      -0.879635    -0.759671    -0.017457      11.89
 O      -2.280577    -0.532339     0.237030     128.07
 C      -0.235241    -1.278673    -1.182994      59.35
 H      -0.847077    -1.996025    -1.941352      22.03
 C       1.995769    -0.520277    -0.293127      19.05
 C       3.458023    -0.096462    -0.711313      77.60
 H       3.311539    -0.210453    -1.828430      21.38
 O       3.824648     1.202610    -0.318917     228.64
 H       4.139112     1.048945     0.668118      21.00
 C       4.406969    -1.131624     0.030654      96.79
 H       4.573468    -0.803728     1.077856      25.27
 O       4.041741    -2.605869     0.086436     253.25
 H       3.987499    -2.740734    -0.993148      25.91
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 C       5.881838    -1.008999    -0.406333     119.67
 O       6.651654     0.235574    -0.343168     322.43
 H       6.878992     0.538730     0.563597      34.44
 H       5.829708    -1.196370    -1.517530      31.55
 H       6.408572    -1.721754    -0.013012      32.12
55
name= lig-ACN-Water-frame_741
 C      -4.197335     1.491137    -2.672235      73.62
 H      -4.174615     0.696693    -3.283724      24.08
 C      -4.280564     2.627060    -0.608703      78.94
 H      -4.405377     2.505432     0.435598      24.08
 C      -3.686751     3.882468    -1.135251     -16.70
 O      -3.416703     4.982843    -0.367999     203.46
 C      -3.240912     4.917893     1.042080     103.13
 H      -2.355772     5.657822     1.512742      23.60
 H      -2.876394     3.840894     1.508161      24.71
 H      -4.125203     5.154025     1.464843      25.53
 C      -3.767666     4.050349    -2.664160      -7.85
 O      -3.392391     5.207072    -3.272775     111.67
 H      -3.310151     5.955802    -2.522363      21.82
 C      -3.804794     2.707862    -3.375550      23.78
 H      -3.842877     2.649433    -4.492186      17.02
 C      -4.501008     1.472243    -1.313970      57.02
 C      -4.574512     0.100950    -0.711976      88.47
 H      -5.141631    -0.357357    -1.425549      27.05
 O      -5.233039    -0.067817     0.566793     244.37
 H      -4.528577    -0.085020     1.243698      26.27
 C      -3.175245    -0.862472    -0.856448      90.46
 H      -2.713297    -0.596173    -1.676183      29.39
 C      -3.410071    -2.415525    -0.889047     115.29
 O      -4.375151    -2.835847    -1.794940     176.37
 H      -3.833462    -3.522758    -2.424495      24.07
 H      -3.770743    -2.801743     0.080800      26.60
 H      -2.517199    -2.885566    -1.412490      22.66
 C       1.121925    -1.116341    -1.346425      30.77
 H       1.649902    -1.522114    -2.176261      22.30
 C       1.370208    -0.179553     0.763501     106.45
 H       1.794087     0.140188     1.794012      15.59
 C      -0.000686    -0.131530     0.965586       9.49
 O      -0.804588     0.462930     2.044114     178.19
 C      -0.138686     0.599627     3.403799     104.41
 H       0.074216     1.800125     3.586001      22.97
 H      -0.747497     0.311983     4.113196      27.89
 H       0.636371    -0.234200     3.458326      25.93
 C      -0.868420    -0.624684    -0.034293       9.56
 O      -2.230809    -0.562126     0.195562     152.77
 C      -0.256014    -1.222266    -1.158962      68.71
 H      -0.933176    -1.684024    -1.943649      23.18
 C       1.946727    -0.576013    -0.464702      54.76
 C       3.380418    -0.247768    -0.728527      69.47
 H       3.693297    -0.027923    -1.832834      19.14
 O       3.907825     1.193971    -0.314853     148.81
 H       4.126548     1.301350     0.661136      25.24
 C       4.447445    -1.148609    -0.023901     115.28
 H       4.243406    -0.928237     0.973399      27.22
 O       4.008305    -2.513420     0.050349     334.22
 H       4.331398    -3.073388    -0.769188      28.61
 C       5.928862    -1.076396    -0.521710     123.18
 O       6.683921     0.300060    -0.301577     294.28
 H       7.129779     0.138330     0.616684      30.31
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 H       6.033481    -1.247600    -1.573501      32.29
 H       6.330564    -1.797610     0.006534      31.15
55
name= lig-ACN-Water-frame_742
 C      -4.236147     1.532585    -2.728694       5.01
 H      -4.378022     0.651440    -3.224749      21.89
 C      -4.193905     2.741157    -0.538192      10.06
 H      -4.397048     2.714539     0.576205      18.63
 C      -3.798266     3.865439    -1.182905       3.80
 O      -3.334487     4.968358    -0.375955     215.59
 C      -3.336112     4.830661     1.080269      95.40
 H      -2.458300     5.731610     1.403659      21.98
 H      -3.095970     3.735781     1.352996      25.05
 H      -4.219526     5.100593     1.483650      23.94
 C      -3.658895     3.898697    -2.619213       3.42
 O      -3.513894     5.205373    -3.229279     165.17
 H      -3.402167     6.011899    -2.613619      20.82
 C      -3.836411     2.728134    -3.352626      84.24
 H      -3.508643     2.698535    -4.338766      28.44
 C      -4.583926     1.558578    -1.373084       2.60
 C      -4.476759    -0.015094    -0.785410      75.00
 H      -5.088653    -0.579865    -1.352589      26.67
 O      -5.263051    -0.112334     0.496077     185.14
 H      -4.734734    -0.011530     1.367568      24.31
 C      -3.093769    -0.912311    -0.931664      85.41
 H      -2.761031    -0.712548    -1.850885      29.19
 C      -3.338503    -2.464357    -0.938101     113.30
 O      -4.383315    -2.834632    -1.918060     260.10
 H      -4.038668    -3.129802    -2.781714      27.17
 H      -3.585727    -2.778556     0.144885      25.58
 H      -2.289669    -2.910970    -0.939902      24.43
 C       1.131855    -1.270704    -1.452839      33.96
 H       1.413674    -1.717317    -2.430212      17.43
 C       1.394254     0.054068     0.771168      42.89
 H       2.283429     0.607696     1.295751      13.30
 C      -0.052169    -0.134175     1.040810      19.61
 O      -0.736405     0.455850     2.020670     220.73
 C      -0.226089     0.594492     3.293280     134.71
 H       0.318059     1.568009     3.589993      25.65
 H      -0.940538     0.381799     3.866802      29.49
 H       0.779118     0.015493     3.431415      24.73
 C      -0.863416    -0.527237    -0.058012      16.97
 O      -2.258480    -0.575104     0.207756     145.67
 C      -0.316882    -1.213988    -1.210232      50.02
 H      -0.872091    -1.560423    -2.042156      22.72
 C       1.970380    -0.493069    -0.437176       8.10
 C       3.508192    -0.234956    -0.741300      80.49
 H       3.571655    -0.588947    -1.897505      20.55
 O       3.879048     1.132871    -0.328928     220.37
 H       4.136128     0.983801     0.589837      24.32
 C       4.425366    -1.148330     0.019400     100.55
 H       4.635296    -0.767224     0.961424      27.31
 O       3.996982    -2.526150    -0.037019     319.00
 H       4.314031    -2.824940    -0.871946      31.56
 C       6.104170    -1.022555    -0.573861     110.68
 O       6.654727     0.207501    -0.298925     324.25
 H       6.991555     0.361752     0.686962      29.47
 H       6.153242    -1.267699    -1.595979      33.62
 H       6.626236    -1.741137    -0.101082      32.10
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name= lig-ACN-Water-frame_743
 C      -4.313314     1.625471    -2.784829      50.81
 H      -4.272886     0.746213    -3.429243      27.14
 C      -4.262224     2.622477    -0.537477      68.32
 H      -4.250980     2.667164     0.667266      21.38
 C      -3.854289     3.898647    -1.098335      -5.29
 O      -3.286604     4.962808    -0.480014     165.77
 C      -3.425091     4.766396     1.089024      90.75
 H      -2.551697     5.657740     1.512287      22.42
 H      -2.963262     3.865576     1.497863      25.33
 H      -4.382267     4.935708     1.441293      24.90
 C      -3.579553     3.932091    -2.537236       4.01
 O      -3.608240     5.096035    -3.219017     174.59
 H      -3.774797     5.812081    -2.617207      24.08
 C      -3.817656     2.816481    -3.388945      39.93
 H      -3.575108     2.917555    -4.352049      24.55
 C      -4.381088     1.440327    -1.288007     -35.20
 C      -4.550120    -0.105801    -0.842176      79.97
 H      -5.132608    -0.537022    -1.577550      24.03
 O      -5.212077    -0.168280     0.437051     186.32
 H      -4.572739     0.312470     1.018113      28.02
 C      -3.161787    -0.852544    -0.957544      81.19
 H      -2.689896    -0.440342    -1.764931      28.18
 C      -3.301431    -2.449538    -0.940674     100.15
 O      -4.369382    -2.841377    -1.997376     250.08
 H      -3.927883    -2.659413    -2.804961      30.45
 H      -4.003091    -2.655285    -0.026372      23.00
 H      -2.400127    -3.055707    -1.131261      24.14
 C       1.119335    -1.221497    -1.338117      22.46
 H       1.656447    -1.789701    -2.159166      21.26
 C       1.376155     0.173721     0.657929      87.01
 H       1.757278     1.009464     1.338508      17.40
 C       0.038987    -0.018793     0.894689       4.70
 O      -0.748194     0.489020     1.999000     182.85
 C      -0.161583     0.587433     3.349053     122.17
 H      -0.037069     1.696303     3.356363      23.36
 H      -0.869852     0.447676     4.002172      28.58
 H       0.527445    -0.270188     3.512960      25.99
 C      -0.815176    -0.627519    -0.092437     -10.44
 O      -2.266700    -0.556733     0.182783     123.32
 C      -0.246301    -1.188115    -1.247283      78.53
 H      -0.913569    -1.691428    -1.765480      24.99
 C       1.939294    -0.498445    -0.491012      43.79
 C       3.520234    -0.244621    -0.720809      71.32
 H       3.769065    -0.112648    -1.929765      17.33
 O       3.810239     1.082513    -0.379879     207.55
 H       4.280239     1.207169     0.481996      24.47
 C       4.666637    -1.216334     0.009019      98.40
 H       4.537562    -1.127179     1.101713      26.61
 O       4.031561    -2.570223    -0.127948     392.37
 H       3.925000    -2.623997    -1.057520      29.42
 C       6.089557    -1.114766    -0.509722     125.26
 O       6.678636     0.236452    -0.313562     320.57
 H       6.729548     0.359535     0.650132      33.49
 H       6.096836    -1.169522    -1.576381      33.55
 H       6.648457    -1.864096    -0.143882      31.48
55
name= lig-ACN-Water-frame_744
 C      -4.220808     1.625616    -2.741857      56.73
 H      -4.484446     0.818659    -3.531761      25.40
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 C      -4.258086     2.501420    -0.532014      57.39
 H      -4.441741     2.151105     0.621378      22.22
 C      -3.797293     3.740498    -1.102389      15.37
 O      -3.320507     4.930823    -0.362284     186.76
 C      -3.409574     4.813662     0.994103     107.61
 H      -3.018617     5.865459     1.659752      23.11
 H      -3.022100     3.904228     1.261003      29.42
 H      -4.469193     4.763012     1.189755      25.63
 C      -3.723847     3.935830    -2.483085      15.29
 O      -3.643947     5.135469    -3.232346     173.99
 H      -3.390749     5.942805    -2.693191      23.47
 C      -3.826652     2.829445    -3.332633      53.64
 H      -4.008644     2.976157    -4.305949      22.55
 C      -4.216199     1.342299    -1.422404       7.87
 C      -4.583043    -0.031775    -0.906986      95.35
 H      -5.268080    -0.602639    -1.517253      24.25
 O      -5.119871    -0.201634     0.393090     177.88
 H      -4.586119     0.064753     1.142917      26.63
 C      -3.175019    -0.864262    -0.951040      69.05
 H      -2.777233    -0.659037    -1.931686      27.76
 C      -3.502306    -2.367102    -1.015456     124.33
 O      -4.309367    -2.771316    -1.996235     255.39
 H      -3.851120    -3.086623    -2.935289      22.14
 H      -3.733149    -2.754727     0.081515      24.73
 H      -2.518187    -2.879012    -1.096558      24.30
 C       1.240120    -1.175824    -1.288759      67.11
 H       1.692087    -1.836564    -2.114709      18.12
 C       1.350344     0.286452     0.530518      56.70
 H       2.012867     0.816909     1.216228      19.74
 C      -0.088862     0.107319     0.791580      15.46
 O      -0.746333     0.491330     1.946879     151.44
 C      -0.128882     0.628869     3.392443     109.65
 H       0.540561     1.439220     3.668195      23.88
 H      -0.860784     0.474494     3.972202      26.75
 H       0.791407     0.021709     3.545356      24.43
 C      -0.901908    -0.682378    -0.072493      24.20
 O      -2.208626    -0.521699     0.130420     157.18
 C      -0.266451    -1.249242    -1.208490      67.07
 H      -0.539295    -1.803772    -1.994180      22.63
 C       2.092228    -0.436711    -0.426778      38.78
 C       3.572605    -0.306168    -0.675546      81.14
 H       3.751300    -0.620131    -1.870248      18.61
 O       3.770008     1.204904    -0.391288     245.42
 H       3.974231     1.142990     0.634411      21.94
 C       4.582872    -1.317939     0.003691     104.82
 H       4.733664    -1.090091     1.130203      24.17
 O       4.112249    -2.617436    -0.225799     335.90
 H       4.188786    -2.937099    -1.172624      27.40
 C       6.090033    -1.189798    -0.520167     112.41
 O       6.687237     0.264080    -0.308454     259.19
 H       7.054112     0.280557     0.575800      31.48
 H       6.094648    -1.463470    -1.589515      36.16
 H       6.663119    -1.870326     0.008416      33.73
55
name= lig-ACN-Water-frame_745
 C      -4.036166     1.493401    -2.902151      35.49
 H      -4.355313     0.513112    -3.573891      20.07
 C      -4.078353     2.397790    -0.558732      80.92
 H      -4.379351     2.460048     0.586543      20.19
 C      -3.696035     3.687137    -1.028046      -3.80
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 O      -3.391831     4.840077    -0.404418     190.90
 C      -3.509039     4.796180     1.073508     104.83
 H      -2.997608     5.934493     1.344631      23.94
 H      -2.846973     4.226001     1.548595      29.73
 H      -4.506217     4.611843     1.581570      25.06
 C      -3.862101     3.970639    -2.501046       3.18
 O      -3.635997     5.224107    -3.195839      72.74
 H      -3.411151     6.005905    -2.502302      21.02
 C      -3.977399     2.833746    -3.310853      47.19
 H      -3.998758     3.011950    -4.373898      22.85
 C      -4.286660     1.369560    -1.401185      23.56
 C      -4.407057    -0.041312    -0.920972      97.03
 H      -5.151666    -0.460401    -1.651926      25.71
 O      -5.085023    -0.179434     0.424685     161.92
 H      -4.286029    -0.232136     1.035427      26.13
 C      -3.224011    -0.883084    -1.046932      95.70
 H      -2.646749    -0.696976    -1.986999      26.78
 C      -3.448907    -2.366637    -0.886361     102.87
 O      -4.408845    -2.702798    -2.093621     167.84
 H      -3.786015    -3.472652    -2.553690      23.11
 H      -4.133818    -2.632156     0.016646      24.81
 H      -2.467709    -2.864335    -1.003430      24.32
 C       1.282445    -1.209014    -1.290125      57.18
 H       1.713405    -1.658181    -2.233244      22.30
 C       1.312548     0.362959     0.573783      56.99
 H       1.729690     0.973351     1.322369      22.97
 C      -0.064243     0.168623     0.784546     -10.58
 O      -0.705406     0.570246     2.021665     163.82
 C      -0.011742     0.621217     3.272493     125.77
 H       0.249459     1.705463     3.317639      23.70
 H      -0.721023     0.600238     3.932675      29.07
 H       0.473861    -0.302783     3.274982      27.18
 C      -0.864045    -0.619298    -0.175516     -27.58
 O      -2.336573    -0.519578     0.058769      94.43
 C      -0.068032    -1.352137    -1.154795      74.30
 H      -0.787266    -1.764878    -1.820280      24.95
 C       2.050641    -0.436373    -0.409690      21.18
 C       3.601317    -0.245835    -0.632817      76.64
 H       3.747345    -0.295131    -1.867438      20.61
 O       3.799123     1.216178    -0.379985     253.93
 H       4.145139     1.412693     0.548515      22.64
 C       4.533461    -1.288841     0.042722      83.68
 H       4.456961    -1.143419     1.235520      22.93
 O       4.179463    -2.736300    -0.231246     292.19
 H       4.244938    -2.575212    -1.254483      25.15
 C       6.120709    -1.111682    -0.489609     112.73
 O       6.663510     0.147436    -0.346647     290.57
 H       7.117439     0.209801     0.567298      28.90
 H       6.356185    -1.364899    -1.564337      32.57
 H       6.641247    -1.820253     0.113837      30.16
55
name= lig-ACN-Water-frame_746
 C      -4.018602     1.480515    -2.862632      28.93
 H      -3.744886     0.630952    -3.735300      19.93
 C      -3.893473     2.463264    -0.559100      41.39
 H      -3.830557     2.160839     0.524955      19.83
 C      -3.718944     3.711979    -1.200795      15.29
 O      -3.467649     4.787411    -0.331100     232.29
 C      -3.511810     4.830364     1.195022      83.12
 H      -3.525860     6.038715     1.323488      22.51
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 H      -2.798328     4.271429     1.554351      30.50
 H      -4.618443     4.500403     1.471783      23.28
 C      -3.869188     3.948847    -2.535386      14.67
 O      -3.643245     5.181679    -3.074934     203.94
 H      -3.838496     6.028150    -2.493095      21.43
 C      -4.114503     2.820882    -3.427857      38.53
 H      -3.888516     3.064530    -4.523771      24.71
 C      -4.227500     1.327373    -1.498000      24.32
 C      -4.485303    -0.081655    -0.916836      95.80
 H      -5.219499    -0.741230    -1.545011      23.63
 O      -4.981076    -0.149605     0.418361     209.34
 H      -4.304935    -0.071527     1.173089      23.83
 C      -3.108153    -0.954152    -1.096942      75.12
 H      -2.765436    -0.703164    -2.215149      24.23
 C      -3.530882    -2.445134    -0.913681     109.18
 O      -4.464244    -2.662102    -2.055552     209.87
 H      -4.016832    -3.084096    -2.875744      24.99
 H      -4.097148    -2.490549     0.111376      25.11
 H      -2.836403    -3.284717    -0.828989      25.60
 C       1.354578    -1.249553    -1.299737      48.60
 H       1.983437    -1.752060    -2.050718      15.66
 C       1.327749     0.323830     0.663740      57.36
 H       1.880526     1.064500     1.149830      19.76
 C      -0.078111     0.143604     0.845237      16.32
 O      -0.731385     0.638020     1.926691     217.14
 C       0.065692     0.629513     3.154317     135.76
 H       0.918643     1.388265     3.229145      24.40
 H      -0.546220     0.649594     3.899327      29.56
 H       0.854823     0.001180     3.358598      27.39
 C      -0.815932    -0.478517    -0.157124      10.67
 O      -2.259867    -0.524654    -0.011212     151.82
 C      -0.153022    -1.342566    -1.105693      53.47
 H      -0.478040    -2.111754    -1.876736      20.73
 C       1.987380    -0.358885    -0.385978      20.25
 C       3.478018    -0.130225    -0.633799      75.45
 H       3.772266    -0.291219    -1.816802      19.37
 O       3.906345     1.195171    -0.328722     252.23
 H       4.406780     1.146226     0.475164      23.35
 C       4.609626    -1.263624     0.032456      76.31
 H       4.435905    -1.293397     1.232269      21.55
 O       4.242557    -2.702078    -0.208116     302.43
 H       3.906737    -3.114952    -1.055069      27.35
 C       6.033582    -1.178833    -0.377888     102.37
 O       6.718277     0.144489    -0.347749     278.03
 H       6.754704     0.384993     0.676225      28.36
 H       5.820979    -1.493312    -1.446972      29.06
 H       6.647059    -1.942998     0.093539      29.56
55
name= lig-ACN-Water-frame_747
 C      -4.115584     1.610697    -2.896126      39.80
 H      -4.001291     0.542392    -3.517043      22.58
 C      -3.816361     2.360923    -0.719142      62.92
 H      -3.489717     2.307289     0.268982      19.98
 C      -3.791869     3.682224    -1.090924      -1.38
 O      -3.500245     4.865951    -0.266827     227.10
 C      -3.591750     4.818442     1.136429     112.06
 H      -3.592885     5.870032     1.552937      24.23
 H      -2.794114     4.477006     1.617833      29.99
 H      -4.490399     4.136746     1.628810      24.02
 C      -3.888836     3.867400    -2.608829      13.47
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 O      -3.691123     5.114353    -3.067378      93.08
 H      -3.372562     5.692904    -2.326468      23.51
 C      -4.059623     2.824978    -3.479822      83.65
 H      -4.122505     2.830179    -4.673286      23.34
 C      -4.057449     1.277631    -1.481679      26.64
 C      -4.434381    -0.128898    -0.945255      70.71
 H      -5.425417    -0.475901    -1.521683      21.01
 O      -4.897097    -0.122106     0.442655     185.93
 H      -4.205917     0.285356     0.983837      25.29
 C      -3.051933    -1.062107    -1.076334      63.74
 H      -2.407381    -0.944108    -2.133165      21.90
 C      -3.644112    -2.515404    -0.989824     116.26
 O      -4.550787    -2.671329    -2.013739     279.43
 H      -4.044200    -2.531015    -2.749360      33.93
 H      -4.294949    -2.573493    -0.071212      23.24
 H      -2.777284    -3.219241    -1.006043      25.32
 C       1.233626    -1.212814    -1.164334      51.95
 H       1.611330    -1.930250    -1.838025      20.80
 C       1.370700     0.263174     0.686218      54.35
 H       1.951978     0.844394     1.393819      16.57
 C      -0.026206     0.128263     0.806374      13.01
 O      -0.752578     0.712373     1.909050     184.32
 C       0.205577     0.665226     3.119875     113.41
 H       0.770578     1.668734     3.036323      20.87
 H      -0.363941     0.812650     3.922424      27.48
 H       0.393667    -0.247112     2.891008      25.71
 C      -0.800521    -0.561130    -0.215135      15.89
 O      -2.100674    -0.501273    -0.060265     152.56
 C      -0.080824    -1.278137    -1.142378      65.98
 H      -0.880139    -1.961374    -1.646687      15.08
 C       2.023277    -0.316789    -0.395949      59.74
 C       3.525542    -0.189067    -0.651263      68.41
 H       3.524850    -0.348842    -1.840323      20.34
 O       4.028977     1.210147    -0.260700     203.25
 H       4.282987     1.143939     0.710681      22.24
 C       4.442180    -1.275132     0.076640      85.16
 H       4.474842    -0.913754     1.209378      22.61
 O       4.248283    -2.650613    -0.138241     286.23
 H       4.303859    -2.516109    -1.130172      25.88
 C       5.997974    -1.212719    -0.406913      95.43
 O       6.721987     0.125835    -0.318243     259.76
 H       6.955045     0.333809     0.632308      32.07
 H       6.283609    -1.395464    -1.502518      30.23
 H       6.518329    -1.991083     0.248710      29.41
55
name= lig-ACN-Water-frame_748
 C      -4.235388     1.427583    -2.941702      43.50
 H      -4.873380     0.769783    -3.718853      21.18
 C      -3.695456     2.343155    -0.591730      42.72
 H      -3.689537     2.077608     0.372981      20.61
 C      -3.819560     3.728002    -1.111107      10.54
 O      -3.557183     4.871144    -0.381259     200.50
 C      -3.644177     4.753206     1.158747      94.24
 H      -4.050500     5.714478     1.396626      24.95
 H      -2.704536     4.498415     1.470723      28.40
 H      -4.570365     3.954330     1.400748      23.43
 C      -3.875849     3.888835    -2.481632      12.33
 O      -3.724584     5.107827    -3.146648     170.26
 H      -3.458148     5.894577    -2.655584      25.42
 C      -3.981939     2.793020    -3.445785      13.86
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 H      -4.162482     3.169941    -4.597200      18.94
 C      -3.972735     1.257451    -1.578278      18.88
 C      -4.194680    -0.096081    -0.948366      88.35
 H      -4.975365    -0.671306    -1.676338      20.54
 O      -4.803244    -0.074527     0.416867     197.87
 H      -4.147736     0.123583     1.145139      23.63
 C      -3.124464    -1.098969    -1.028788      70.86
 H      -2.702369    -1.052298    -2.230360      20.33
 C      -3.604039    -2.567721    -0.889285      99.89
 O      -4.672968    -2.680201    -2.070286     146.20
 H      -4.242337    -2.824901    -3.015162      25.32
 H      -4.068370    -2.855098     0.047188      25.67
 H      -2.844164    -3.349554    -1.189631      23.53
 C       1.319609    -1.241317    -1.196273      47.07
 H       1.931526    -1.673209    -1.935181      17.35
 C       1.393646     0.253709     0.710545      70.17
 H       1.911344     0.784945     1.589223      14.78
 C       0.000492     0.197453     0.770229      12.51
 O      -0.706796     0.785736     1.929587     238.62
 C       0.157603     0.672977     3.041052     131.98
 H       1.141955     1.279772     3.072700      22.35
 H      -0.363823     0.855153     3.898903      28.03
 H       0.759459    -0.082766     3.348622      27.26
 C      -0.747983    -0.564980    -0.120989      14.68
 O      -2.174966    -0.515644    -0.082215     146.10
 C      -0.165836    -1.293109    -1.184749      84.19
 H      -0.488389    -1.983310    -2.059331      18.45
 C       2.082639    -0.387465    -0.392884      22.22
 C       3.597573    -0.218550    -0.653943      88.79
 H       4.067710    -0.105655    -1.666755      18.97
 O       4.091875     1.152105    -0.241940     233.32
 H       4.291402     1.174172     0.786634      23.45
 C       4.491527    -1.164673     0.079476      79.10
 H       4.225237    -1.203493     1.232600      22.77
 O       4.137314    -2.606717    -0.138216     316.27
 H       4.358268    -3.075611    -0.941580      33.11
 C       6.040925    -1.086465    -0.408222     101.48
 O       6.699432     0.069135    -0.256505     269.30
 H       7.057497    -0.011768     0.614297      32.55
 H       5.935999    -1.611890    -1.425561      31.65
 H       6.478347    -1.903538     0.299449      28.66
55
name= lig-ACN-Water-frame_749
 C      -4.305366     1.462808    -2.972107      55.40
 H      -4.830663     0.617175    -3.478753      22.53
 C      -3.671829     2.348362    -0.649077      69.89
 H      -3.608176     2.128612     0.366362      20.08
 C      -3.703596     3.644989    -1.098208      11.18
 O      -3.652864     4.862171    -0.407656     221.74
 C      -3.740400     4.719273     1.024452     122.18
 H      -4.083016     5.556119     1.474552      26.58
 H      -2.779137     4.522234     1.543919      27.41
 H      -4.403551     3.729154     1.323604      25.26
 C      -3.799505     3.872401    -2.533097      19.71
 O      -3.752360     5.136757    -3.247441     166.83
 H      -3.877737     5.823425    -2.531119      25.31
 C      -4.026061     2.748511    -3.288994      50.15
 H      -4.062787     3.055571    -4.455153      22.86
 C      -3.937287     1.296807    -1.553703       3.76
 C      -4.200244    -0.102036    -0.930125      90.66
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 H      -5.171671    -0.502981    -1.503873      22.19
 O      -4.717231    -0.017971     0.360284     232.27
 H      -3.990579    -0.183033     1.067613      22.54
 C      -3.056823    -1.122503    -1.025411      74.05
 H      -2.563433    -1.000499    -2.206109      22.28
 C      -3.626879    -2.645883    -0.959353     102.06
 O      -4.694670    -2.690612    -2.026559     185.57
 H      -4.243698    -3.503025    -2.579299      24.62
 H      -4.103727    -2.794951    -0.030109      26.50
 H      -2.678530    -3.314427    -1.090875      24.36
 C       1.407641    -1.231943    -1.349065      50.52
 H       1.738582    -1.722109    -2.249600      20.01
 C       1.449003     0.234417     0.660825      54.71
 H       2.203389     0.995925     1.171041      15.32
 C      -0.016193     0.240439     0.797968      -0.85
 O      -0.584308     0.774672     1.891956     186.09
 C       0.169682     0.709867     3.185818     111.55
 H       0.862843     1.533549     3.096540      22.33
 H      -0.576933     1.184281     3.730432      25.83
 H       0.223452    -0.295242     3.211290      26.00
 C      -0.846923    -0.622214    -0.186343     -13.04
 O      -2.197328    -0.566017     0.002908     159.67
 C       0.003887    -1.327741    -1.174624      53.41
 H      -0.707886    -1.732613    -1.931941      19.34
 C       2.131967    -0.447376    -0.345577      22.69
 C       3.677703    -0.133684    -0.641670      80.90
 H       3.517682    -0.389624    -1.655329      23.12
 O       4.097905     1.134214    -0.232014     245.50
 H       4.463110     0.983501     0.749705      22.36
 C       4.579454    -1.253977     0.061291      93.81
 H       4.617171    -0.949593     1.188252      25.31
 O       3.989678    -2.578109    -0.112197     284.03
 H       4.198845    -2.694736    -1.098170      29.47
 C       5.954282    -1.210125    -0.320905     105.82
 O       6.769268     0.115861    -0.188366     169.84
 H       6.952265     0.360265     0.771382      32.86
 H       6.080192    -1.157428    -1.453902      30.90
 H       6.674532    -2.069130    -0.006173      29.57
55
name= lig-ACN-Water-frame_750
 C      -4.252099     1.525529    -2.776189      52.29
 H      -4.238682     0.775036    -3.490634      25.44
 C      -3.665445     2.329120    -0.729878      41.47
 H      -3.353459     2.184111     0.351894      18.69
 C      -3.555329     3.711969    -1.225886      11.05
 O      -3.744429     4.841240    -0.409050     197.33
 C      -3.816202     4.671512     0.996806     122.28
 H      -4.266871     5.500024     1.272299      27.05
 H      -2.728685     4.564602     1.355585      25.50
 H      -4.532218     3.763280     1.295536      25.60
 C      -3.721744     3.885800    -2.624707      19.98
 O      -3.783931     5.086867    -3.236071     162.38
 H      -3.644819     5.976069    -2.665203      20.59
 C      -4.133461     2.797224    -3.444541      46.26
 H      -4.265257     2.841733    -4.573134      24.94
 C      -4.002308     1.207094    -1.469932      42.77
 C      -4.344236    -0.115166    -1.004955      83.61
 H      -5.224669    -0.539619    -1.641275      22.28
 O      -4.699464     0.001726     0.412653     188.92
 H      -3.896874     0.215139     1.000881      20.35
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 C      -3.062849    -1.135650    -1.100370      63.97
 H      -2.221497    -0.988493    -2.029980      20.54
 C      -3.621275    -2.573227    -0.993197     116.42
 O      -4.609257    -2.785067    -1.960412     302.12
 H      -4.525477    -3.506056    -2.513751      32.29
 H      -4.052475    -2.711974    -0.020125      24.73
 H      -2.910642    -3.466022    -1.225011      22.56
 C       1.396023    -1.159337    -1.369693      44.40
 H       1.952679    -1.685589    -2.178412      16.66
 C       1.426980     0.231849     0.547274      59.43
 H       1.776946     1.049659     1.315194      18.23
 C       0.108330     0.086557     0.726188      18.33
 O      -0.570580     0.804489     1.855844     142.98
 C       0.079728     0.793498     3.280731     124.86
 H       1.069322     1.040443     3.510256      25.77
 H      -0.631914     1.138832     4.062116      26.00
 H       0.302214    -0.149463     3.670104      27.88
 C      -0.626085    -0.594787    -0.145930       8.03
 O      -2.139651    -0.720211     0.083521     114.50
 C       0.013673    -1.292529    -1.158267      61.07
 H      -0.392567    -1.970485    -1.840336      20.10
 C       2.177457    -0.500410    -0.443924      44.69
 C       3.635152    -0.237510    -0.609441      96.41
 H       4.069239    -0.108308    -1.518471      19.27
 O       4.093566     1.177683    -0.262225     252.89
 H       4.331668     1.299493     0.728002      22.31
 C       4.504620    -1.278441     0.139314      83.94
 H       4.431809    -1.214142     1.277129      22.36
 O       3.905191    -2.531356    -0.130309     308.66
 H       3.511966    -2.663533    -1.078076      26.47
 C       6.181632    -1.242225    -0.456997      71.82
 O       6.759256     0.100389    -0.106079     251.22
 H       6.854847     0.083780     0.954099      27.68
 H       6.123525    -1.380091    -1.566342      31.11
 H       6.588095    -2.226309     0.101661      27.79
55
name= lig-ACN-Water-frame_751
 C      -4.173390     1.513892    -2.907080      53.02
 H      -4.417127     0.734626    -3.443913      24.34
 C      -3.567220     2.425058    -0.657736      42.09
 H      -3.476408     2.365027     0.532171      16.67
 C      -3.525975     3.648996    -1.326191       2.28
 O      -3.780062     4.810025    -0.526247     148.09
 C      -3.896029     4.658543     1.031907     105.36
 H      -4.258768     5.479648     1.391907      27.40
 H      -2.873164     4.432888     1.660929      24.92
 H      -4.544055     3.780178     1.280066      26.62
 C      -3.729770     3.869043    -2.723156      16.77
 O      -3.791519     5.177232    -3.237199     183.91
 H      -3.364850     5.811998    -2.564932      22.81
 C      -4.160814     2.801727    -3.512801      53.37
 H      -4.434085     2.942873    -4.507887      23.02
 C      -4.067363     1.326284    -1.481224       5.58
 C      -4.275345    -0.192489    -0.912424      90.15
 H      -5.115764    -0.757937    -1.401132      22.82
 O      -4.791986    -0.054404     0.419618     222.77
 H      -4.164274     0.253244     1.078669      23.89
 C      -3.055433    -1.101057    -1.104390      43.64
 H      -2.766488    -0.906297    -2.305108      20.49
 C      -3.511617    -2.570732    -0.933130      93.21
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 O      -4.636879    -2.843177    -1.966111     279.43
 H      -4.060938    -3.338180    -2.591179      27.57
 H      -3.902435    -2.657803     0.084774      24.51
 H      -2.516547    -3.154381    -0.953472      23.24
 C       1.420543    -1.170493    -1.383640      14.72
 H       1.829078    -1.729630    -2.304798      18.24
 C       1.556022     0.271624     0.529533      48.01
 H       2.319533     0.794655     1.208230      17.76
 C       0.119601     0.071057     0.904950     -10.40
 O      -0.508608     0.810716     1.882925     195.93
 C       0.000155     0.739686     3.300980     122.33
 H       0.783676     1.356864     3.175043      24.86
 H      -0.738993     1.596374     3.595251      23.57
 H      -0.098359    -0.210958     3.631240      27.66
 C      -0.738822    -0.713359    -0.145483     -12.02
 O      -2.000359    -0.909983     0.101570     118.98
 C      -0.009764    -1.331201    -1.254195      41.84
 H      -0.547040    -1.990449    -1.782722      18.96
 C       2.187333    -0.324098    -0.519743      25.02
 C       3.770960    -0.193260    -0.599638      96.79
 H       3.811929    -0.512266    -1.563286      24.09
 O       4.035143     1.210109    -0.277727     296.45
 H       4.176940     1.158800     0.662465      24.55
 C       4.572160    -1.299794     0.102098      82.91
 H       4.587964    -1.165539     1.202935      24.52
 O       3.841441    -2.579512    -0.147235     327.53
 H       3.635343    -2.547093    -1.117617      26.36
 C       6.158317    -1.219146    -0.450585     103.93
 O       6.716532    -0.029448    -0.074502     276.10
 H       7.189566    -0.113825     0.817022      30.17
 H       6.243029    -1.398467    -1.524743      32.76
 H       6.969345    -1.996069     0.059964      26.50
55
name= lig-ACN-Water-frame_752
 C      -4.198546     1.431913    -2.987091      51.88
 H      -4.690750     0.763058    -3.448452      23.14
 C      -3.565635     2.395085    -0.734455      65.22
 H      -3.589165     2.280987     0.472918      19.95
 C      -3.614140     3.672761    -1.277026     -12.17
 O      -3.743627     4.816944    -0.524043     174.46
 C      -3.971618     4.655425     0.924328     112.97
 H      -4.236625     5.576350     1.188723      27.14
 H      -2.856448     4.316387     1.355744      24.11
 H      -4.741581     3.941862     1.146633      27.05
 C      -3.780314     3.905942    -2.750379       9.02
 O      -3.754174     5.263414    -3.220093     144.53
 H      -3.757255     5.898649    -2.502884      24.14
 C      -4.088810     2.772792    -3.556024      48.06
 H      -4.290160     2.898688    -4.524261      26.72
 C      -3.992298     1.343735    -1.534317      13.74
 C      -4.171014    -0.031473    -0.811556      99.49
 H      -4.847709    -0.412942    -1.567137      26.87
 O      -4.922198    -0.143208     0.440636     159.60
 H      -4.329669    -0.083545     1.222312      24.97
 C      -3.044194    -1.098648    -0.995460      76.41
 H      -2.360964    -0.830385    -1.957070      25.58
 C      -3.465272    -2.560422    -0.901417     105.28
 O      -4.496201    -2.929485    -1.911833     203.34
 H      -4.129364    -2.887589    -2.932790      26.45
 H      -4.022701    -2.823491     0.045045      25.48
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 H      -2.661690    -3.318969    -1.146511      24.37
 C       1.388330    -1.158176    -1.437465      69.95
 H       1.929933    -1.648764    -2.334243      18.30
 C       1.545548     0.277160     0.664592      51.91
 H       2.077492     0.888597     1.408513      17.39
 C       0.178097     0.031759     0.830440      13.34
 O      -0.515104     0.746935     1.874818     231.55
 C      -0.104853     0.829044     3.196425     134.43
 H       0.887792     0.930956     3.516483      26.82
 H      -0.840392     1.420531     3.995338      24.29
 H      -0.180776    -0.071437     3.738699      28.54
 C      -0.548834    -0.766394    -0.075348       2.39
 O      -2.045896    -1.072992     0.059383     117.92
 C       0.017629    -1.336444    -1.221896      58.88
 H      -0.503586    -1.715030    -1.992555      24.83
 C       2.179045    -0.283164    -0.585595      37.88
 C       3.734621    -0.141160    -0.752066      94.08
 H       4.147064     0.006633    -1.677696      23.29
 O       4.043725     1.197944    -0.285138     223.42
 H       4.603787     1.292899     0.487885      25.15
 C       4.664005    -1.355302     0.056300      83.21
 H       4.720471    -1.180465     1.119133      28.65
 O       3.889608    -2.565356    -0.175492     302.11
 H       4.084187    -2.906596    -1.077781      32.83
 C       6.047390    -1.377726    -0.390326      82.85
 O       6.744611    -0.018241    -0.060505     205.91
 H       7.056800    -0.002879     0.857218      31.04
 H       6.015693    -1.244186    -1.447548      33.83
 H       6.424619    -2.540626    -0.125151      29.99
55
name= lig-ACN-Water-frame_753
 C      -4.259612     1.482555    -2.920206      54.86
 H      -4.452616     0.733027    -3.537867      28.85
 C      -3.646426     2.425548    -0.836769      44.58
 H      -3.376766     2.159159     0.284910      22.27
 C      -3.749577     3.752019    -1.331493      36.92
 O      -3.681562     4.879855    -0.523082     239.21
 C      -4.017696     4.696991     0.796626     121.74
 H      -4.192792     5.620198     1.277070      27.31
 H      -3.134195     4.175785     1.567634      24.76
 H      -4.833437     4.109334     0.942131      28.98
 C      -3.836129     3.950505    -2.661217      15.87
 O      -3.702865     5.228781    -3.191836     178.30
 H      -3.946225     5.923674    -2.506155      25.95
 C      -3.982860     2.757220    -3.552649      26.68
 H      -4.007265     2.836285    -4.589528      20.35
 C      -3.842422     1.245702    -1.609042      17.08
 C      -4.185942    -0.029931    -0.897277      80.10
 H      -4.876518    -0.549394    -1.467064      25.70
 O      -4.951083    -0.132290     0.435399     133.18
 H      -4.300961     0.047816     1.222056      23.14
 C      -2.914877    -1.078750    -0.869958      57.30
 H      -2.530230    -0.944295    -1.987660      25.03
 C      -3.486552    -2.628319    -0.964239     102.68
 O      -4.393837    -3.001546    -1.897919     266.92
 H      -3.991523    -2.649838    -2.753068      29.09
 H      -3.859222    -2.798742     0.132008      24.61
 H      -2.480698    -3.111762    -0.939821      25.65
 C       1.468964    -1.029002    -1.452037      20.68
 H       1.915882    -1.435935    -2.405677      19.87
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 C       1.579075     0.194606     0.607616      62.72
 H       1.992112     0.941047     1.212752      20.51
 C       0.171725     0.013245     0.828960      -6.50
 O      -0.601233     0.687910     1.764344     171.96
 C      -0.126422     0.762660     3.288505     101.53
 H       0.845358     1.150527     3.280366      23.81
 H      -0.873028     1.837021     3.469483      20.72
 H      -0.466591    -0.150422     3.577745      25.48
 C      -0.597054    -0.847765    -0.071944      -7.03
 O      -1.941408    -1.128941     0.199448     165.31
 C       0.091095    -1.316976    -1.195824      61.14
 H      -0.503718    -1.898553    -1.882147      21.36
 C       2.205623    -0.344019    -0.516021      43.04
 C       3.713063    -0.100208    -0.816746      85.76
 H       3.835850    -0.363246    -1.820164      25.57
 O       4.106254     1.258322    -0.281636     184.66
 H       4.726355     0.975080     0.506058      22.50
 C       4.472305    -1.267549     0.011487      95.33
 H       4.242686    -1.071048     1.011367      27.90
 O       3.999148    -2.577560    -0.174240     287.72
 H       4.095333    -2.767394    -1.208303      25.84
 C       6.033904    -1.401932    -0.472533      88.98
 O       6.765209    -0.129015    -0.048623     241.13
 H       6.771230    -0.115658     0.940713      31.11
 H       6.116313    -1.612409    -1.528871      32.27
 H       6.774101    -2.221776     0.147006      27.52
55
name= lig-ACN-Water-frame_754
 C      -4.180913     1.542066    -2.997437      50.70
 H      -4.285494     0.709844    -3.652319      23.29
 C      -3.674751     2.454276    -0.795664      56.15
 H      -3.346629     2.482701     0.258435      18.31
 C      -3.828006     3.729649    -1.286690       0.03
 O      -3.600732     4.959352    -0.600465     214.47
 C      -4.108690     4.752064     0.890623      90.97
 H      -4.108480     5.803010     1.299531      24.45
 H      -3.284628     3.967161     1.408582      22.44
 H      -5.008638     4.338121     0.808161      28.61
 C      -3.877628     3.927178    -2.762405      22.16
 O      -3.669464     5.181869    -3.208270     158.21
 H      -3.470499     5.817821    -2.390396      20.26
 C      -3.954007     2.826565    -3.479304      69.30
 H      -3.840294     2.973256    -4.587891      22.02
 C      -3.881012     1.288105    -1.573869       0.93
 C      -4.155053    -0.281570    -0.879686      89.85
 H      -4.775170    -0.731322    -1.551955      23.87
 O      -4.859926     0.003326     0.341938     235.80
 H      -4.231075     0.315104     1.075499      21.87
 C      -2.944410    -1.179420    -0.897774      52.97
 H      -2.194333    -0.852490    -1.662723      21.05
 C      -3.300452    -2.612744    -0.799434      98.41
 O      -4.367199    -3.032076    -1.970209     235.16
 H      -3.932290    -3.157526    -2.773862      29.46
 H      -4.046367    -2.908775     0.073891      22.41
 H      -2.540802    -3.347778    -0.983048      23.79
 C       1.466127    -0.985536    -1.481321      40.79
 H       1.878240    -1.256274    -2.451076      19.60
 C       1.538071     0.194475     0.618547      61.30
 H       2.178610     0.772696     1.176566      19.04
 C       0.119052    -0.062980     0.815195      18.21
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 O      -0.674757     0.655058     1.747562     164.25
 C      -0.188183     0.758031     3.163797     106.60
 H       0.810191     0.833134     3.208097      25.10
 H      -0.844247     1.825804     3.690589      21.48
 H      -0.351329    -0.028355     3.954919      25.47
 C      -0.566521    -0.867022    -0.068846      15.13
 O      -1.865016    -1.120226     0.367299     120.15
 C       0.128385    -1.341662    -1.230744      36.69
 H      -0.257899    -2.160836    -1.931392      16.00
 C       2.264883    -0.336751    -0.489536      61.50
 C       3.660654    -0.098161    -0.765488      90.20
 H       3.834687     0.113093    -1.792226      20.33
 O       4.195953     1.220441    -0.355410     235.28
 H       4.562924     1.270207     0.592533      23.97
 C       4.476122    -1.179275    -0.064923     105.87
 H       4.504153    -0.896268     0.920220      23.24
 O       3.986560    -2.596589    -0.187625     207.39
 H       3.822035    -2.805859    -1.233892      26.12
 C       6.014507    -1.286735    -0.379412      76.71
 O       6.791485    -0.233028    -0.099836     283.17
 H       6.955370    -0.124327     0.915611      30.70
 H       6.259580    -1.457605    -1.431208      29.39
 H       6.159395    -2.412745     0.284256      27.25
55
name= lig-ACN-Water-frame_755
 C      -3.985932     1.483473    -2.966993      39.08
 H      -4.246451     0.645697    -3.717595      22.33
 C      -3.714338     2.403515    -0.686037      28.87
 H      -3.608784     2.185614     0.313874      19.60
 C      -3.804598     3.794493    -1.299390      12.17
 O      -3.586696     4.941741    -0.537115     258.99
 C      -4.147440     4.855624     0.834158     103.18
 H      -3.978338     5.937836     1.332810      23.81
 H      -3.511183     4.110942     1.567258      23.23
 H      -5.132861     4.590175     0.909238      26.38
 C      -3.866583     3.961870    -2.641841       7.75
 O      -3.616949     5.211853    -3.261153     205.78
 H      -3.356785     5.890611    -2.596378      23.27
 C      -3.990435     2.813903    -3.619914      29.40
 H      -3.934394     2.980258    -4.808726      21.66
 C      -4.013492     1.247182    -1.554915      16.65
 C      -4.086690    -0.181430    -0.940989      98.14
 H      -4.753389    -0.760891    -1.452311      25.94
 O      -4.768123     0.084972     0.278410     234.30
 H      -4.154656     0.152720     1.014886      25.12
 C      -2.806665    -1.285472    -0.803092      70.26
 H      -2.376390    -1.165824    -1.784127      23.24
 C      -3.314327    -2.792639    -0.835794      96.61
 O      -4.253124    -3.004423    -1.965218     301.99
 H      -3.676895    -3.655752    -2.484478      26.12
 H      -3.750970    -2.868005     0.298289      23.03
 H      -2.422402    -3.373886    -0.751275      25.41
 C       1.443154    -0.998060    -1.503812      11.47
 H       1.977251    -1.317219    -2.339550      15.90
 C       1.516883     0.219130     0.704433      72.64
 H       1.807060     0.750534     1.546578      16.80
 C       0.179455    -0.040869     0.833687       2.45
 O      -0.712440     0.609294     1.799943     190.71
 C      -0.191958     0.765637     3.078032     108.95
 H       0.821214     0.872153     3.101106      24.44
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 H      -0.625709     1.957813     3.614457      20.34
 H      -0.699505    -0.143549     3.441418      21.81
 C      -0.520256    -0.918374    -0.070159      -2.25
 O      -1.926062    -1.107662     0.375636     147.10
 C       0.113853    -1.418127    -1.243968      70.48
 H      -0.514748    -1.976380    -2.104592      15.65
 C       2.093897    -0.253067    -0.515521      31.87
 C       3.720125    -0.038252    -0.774827      75.57
 H       3.860264    -0.346826    -1.831226      20.70
 O       4.291192     1.230626    -0.383329     263.90
 H       4.223145     1.225766     0.562485      27.26
 C       4.529344    -1.189535    -0.046724     117.16
 H       4.387358    -1.083480     0.945397      28.13
 O       3.878489    -2.487296    -0.156282     295.27
 H       4.170838    -2.716367    -1.230143      22.17
 C       5.964656    -1.370274    -0.375513      85.73
 O       6.941045    -0.172759    -0.070039     218.98
 H       7.025328    -0.109279     0.910261      32.13
 H       6.009796    -1.606543    -1.473931      31.21
 H       6.483618    -2.399042     0.264548      27.73
55
name= lig-ACN-Water-frame_756
 C      -3.912905     1.496992    -3.004067      53.91
 H      -3.840109     0.452947    -3.627418      21.76
 C      -3.878519     2.401826    -0.732123      83.14
 H      -3.927106     2.320415     0.238280      24.49
 C      -3.702616     3.655206    -1.177550     -12.68
 O      -3.599083     4.882868    -0.440530     210.17
 C      -4.152262     4.997484     0.836926     103.19
 H      -3.903287     6.188987     1.165596      23.23
 H      -3.672535     4.208865     1.551731      24.17
 H      -5.213555     4.890961     0.719334      25.46
 C      -3.787103     3.925155    -2.752854       2.37
 O      -3.569023     5.233282    -3.296218     110.10
 H      -3.829363     5.876641    -2.655309      26.47
 C      -3.968230     2.790359    -3.483358      66.09
 H      -4.101634     2.888120    -4.701078      22.33
 C      -3.919970     1.313840    -1.618733      36.36
 C      -4.015269    -0.087048    -0.988537      81.92
 H      -4.637275    -0.585794    -1.672698      26.17
 O      -4.733908     0.064165     0.338334     188.88
 H      -4.061547     0.215290     1.044007      24.99
 C      -2.796517    -1.317040    -0.831539      75.80
 H      -2.203282    -1.260667    -1.658273      24.44
 C      -3.339908    -2.860830    -0.757931     101.37
 O      -4.075534    -3.019280    -1.906788     267.72
 H      -3.742706    -3.593589    -2.744478      25.81
 H      -4.110039    -3.344559     0.050573      21.78
 H      -2.505994    -3.500844    -0.958542      24.12
 C       1.390093    -1.020628    -1.445350      61.07
 H       1.821793    -1.378124    -2.327858      19.18
 C       1.519650     0.244346     0.724331      57.51
 H       2.291940     0.820371     1.191581      15.63
 C       0.062495    -0.049637     0.854487      15.92
 O      -0.700285     0.570193     1.699648     173.81
 C      -0.179049     0.744061     3.132599      81.57
 H       0.897567     0.734252     3.185276      24.16
 H      -0.770928     1.901642     3.344379      20.85
 H      -0.422035     0.076825     4.081778      23.73
 C      -0.586268    -0.950983    -0.020041      18.54
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 O      -1.917002    -1.091254     0.222106     164.52
 C       0.039586    -1.424141    -1.205380      61.56
 H      -0.615302    -2.015104    -2.046623      17.54
 C       2.192020    -0.103833    -0.511035       3.75
 C       3.717468    -0.096349    -0.753773      78.65
 H       3.891471    -0.080288    -1.895566      23.70
 O       4.312542     1.252987    -0.408650     220.26
 H       4.579052     1.311054     0.542413      27.65
 C       4.393644    -1.173451     0.167629      59.07
 H       4.400768    -0.855745     1.140535      28.57
 O       3.784088    -2.395903    -0.165458     248.07
 H       3.830941    -2.601264    -1.262968      24.24
 C       6.187637    -1.347768    -0.396521      66.47
 O       7.014434    -0.209165    -0.057231     215.45
 H       6.906485    -0.094500     0.878374      33.76
 H       6.347577    -1.462815    -1.533741      29.28
 H       6.727136    -2.367574     0.269731      26.40
55
name= lig-ACN-Water-frame_757
 C      -3.879186     1.458724    -2.986929      43.11
 H      -3.717603     0.676782    -3.967711      21.09
 C      -4.010493     2.427667    -0.732822      45.72
 H      -4.187107     2.248533     0.262449      24.13
 C      -3.665755     3.754131    -1.310403      28.13
 O      -3.547018     4.802339    -0.486699     178.39
 C      -4.204564     5.112383     0.918372      84.90
 H      -3.742210     6.270891     1.136489      23.55
 H      -3.877998     4.483538     1.758851      25.04
 H      -5.380499     5.040523     0.975892      24.30
 C      -3.638587     3.925821    -2.625630      40.26
 O      -3.566182     5.160616    -3.271148     146.17
 H      -3.882586     5.884765    -2.624451      26.11
 C      -3.897850     2.808093    -3.485798      38.39
 H      -4.028997     3.044362    -4.680175      23.43
 C      -3.719574     1.269118    -1.581803       3.44
 C      -4.002802    -0.183381    -0.934768      88.79
 H      -4.832112    -0.623569    -1.500527      24.51
 O      -4.698321    -0.033673     0.327231     193.71
 H      -4.073345     0.396689     1.036864      23.02
 C      -2.924849    -1.319361    -0.945921      80.56
 H      -2.568922    -1.300461    -1.883668      26.39
 C      -3.267968    -2.831504    -0.720956      99.26
 O      -4.073102    -3.075426    -2.008829     276.73
 H      -3.311276    -3.051383    -2.629462      28.28
 H      -3.885917    -2.852886     0.307041      24.15
 H      -2.382120    -3.397093    -0.392768      25.61
 C       1.393408    -0.965393    -1.349265     -25.84
 H       1.821156    -1.308453    -2.269285      17.33
 C       1.522754     0.272436     0.568504      75.14
 H       1.665778     0.900202     1.464411      19.54
 C       0.220663    -0.100400     0.805171      -5.17
 O      -0.729708     0.570443     1.831135     153.92
 C      -0.179343     0.791137     3.155037     101.16
 H       0.944813     0.914941     3.125511      22.82
 H      -0.515308     2.008438     3.596354      21.05
 H      -0.724309    -0.087170     3.737817      21.65
 C      -0.584932    -0.913178    -0.049278      14.48
 O      -1.946897    -1.060669     0.195382     129.85
 C       0.085904    -1.358108    -1.138260      68.62
 H      -0.213484    -2.239618    -1.859428      19.26
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 C       2.144323    -0.218067    -0.564038      58.91
 C       3.712993    -0.010767    -0.630239      95.21
 H       4.051796    -0.413725    -1.701296      21.37
 O       4.300846     1.271207    -0.443276     256.18
 H       4.677578     1.272278     0.554397      23.22
 C       4.511589    -1.159449     0.102460      83.17
 H       4.365940    -1.163766     1.151090      26.22
 O       3.691795    -2.389733    -0.135598     316.44
 H       3.740913    -2.415586    -1.146362      26.56
 C       6.237423    -1.280239    -0.304626      74.91
 O       7.083275    -0.220797    -0.026069     260.05
 H       7.165919     0.015734     0.968578      29.39
 H       6.110302    -1.379621    -1.449858      31.90
 H       6.400431    -2.482167     0.155565      27.61
55
name= lig-ACN-Water-frame_758
 C      -3.752169     1.508143    -2.976732      32.11
 H      -3.992535     0.451584    -3.635534      20.32
 C      -3.937672     2.382270    -0.808173      63.63
 H      -4.251022     2.441848     0.251546      21.36
 C      -3.775042     3.681418    -1.191632      -3.32
 O      -3.510023     4.904550    -0.402129     202.42
 C      -4.176396     5.141310     0.882647      98.39
 H      -3.822669     6.370657     1.077414      23.05
 H      -3.799451     4.501719     1.601452      25.12
 H      -5.396063     5.249582     0.732701      23.07
 C      -3.572130     3.892050    -2.676879       6.70
 O      -3.565450     5.142452    -3.223495     146.62
 H      -3.294410     5.853454    -2.490218      21.07
 C      -3.759209     2.794850    -3.512095      65.89
 H      -3.789973     3.005400    -4.665290      23.51
 C      -3.729038     1.174682    -1.511687      18.38
 C      -4.089043    -0.277864    -0.904302      91.18
 H      -4.817997    -0.673363    -1.682161      22.87
 O      -4.686489    -0.151555     0.333858     283.92
 H      -4.002595    -0.069515     1.132036      19.80
 C      -2.881445    -1.268557    -0.993143      90.76
 H      -2.359730    -1.102302    -1.822338      24.19
 C      -3.350454    -2.657046    -0.781283     106.86
 O      -4.008061    -3.180022    -1.991482     311.53
 H      -3.577084    -3.075182    -2.809110      30.88
 H      -4.215111    -2.756843    -0.004080      23.37
 H      -2.489490    -3.331086    -0.692580      23.93
 C       1.501945    -1.017323    -1.496738      32.54
 H       2.038792    -1.527190    -2.345204      18.37
 C       1.433633     0.361327     0.608961      48.25
 H       2.194406     1.061960     1.093661      16.00
 C       0.066761    -0.044213     0.892565      25.29
 O      -0.639110     0.547189     1.888489     202.01
 C      -0.169125     0.836308     3.173256     108.16
 H       0.968570     0.722914     3.333270      22.40
 H      -0.713155     1.934112     3.594646      21.49
 H      -0.406939     0.029450     4.098024      23.21
 C      -0.621831    -0.816367    -0.071980       5.84
 O      -1.989483    -1.001696     0.175216     191.72
 C       0.146074    -1.413172    -1.174778      42.02
 H      -0.487288    -2.053944    -1.850823      18.19
 C       2.273793    -0.190567    -0.431087      14.66
 C       3.794173    -0.071802    -0.662914      73.73
 H       3.831047    -0.093346    -1.857273      19.18
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 O       4.266012     1.318901    -0.421659     287.43
 H       4.320227     1.472137     0.623261      23.07
 C       4.596550    -1.176344     0.110216      91.77
 H       4.655635    -0.942096     1.189842      22.92
 O       3.732919    -2.375642    -0.148804     283.17
 H       3.854974    -2.689515    -0.982898      31.10
 C       5.968756    -1.317590    -0.274164     101.21
 O       7.176124    -0.185802     0.050264     138.67
 H       7.264971    -0.156130     1.086097      28.92
 H       6.242710    -1.378779    -1.377606      29.19
 H       6.695888    -2.150601     0.296443      25.81
55
name= lig-ACN-Water-frame_759
 C      -3.654311     1.415478    -2.906626      57.29
 H      -3.815052     0.546885    -3.777729      21.86
 C      -3.830521     2.316465    -0.629899      32.25
 H      -3.974113     1.889562     0.467288      17.58
 C      -3.764852     3.710885    -1.221583       0.47
 O      -3.499690     4.930649    -0.417181     249.07
 C      -4.122292     5.180066     0.806949     100.98
 H      -3.788020     6.277866     1.341296      23.37
 H      -3.928545     4.505744     1.552497      25.80
 H      -5.401142     4.924935     0.810514      22.16
 C      -3.629155     3.878084    -2.606439       6.68
 O      -3.501376     5.191631    -3.171483     187.28
 H      -3.302463     5.814707    -2.433412      24.28
 C      -3.558355     2.707642    -3.483813      45.73
 H      -3.538721     2.770905    -4.579127      22.43
 C      -3.908920     1.215234    -1.562937      23.40
 C      -4.089827    -0.199011    -1.033431      77.94
 H      -4.873951    -0.838539    -1.605252      21.53
 O      -4.753910    -0.316800     0.378478     186.13
 H      -4.042843    -0.256428     1.066853      22.89
 C      -2.810417    -1.111664    -0.984792      90.44
 H      -2.318253    -1.030169    -1.856551      24.49
 C      -3.414772    -2.643886    -0.945348      96.95
 O      -4.046014    -3.291635    -1.984086     297.50
 H      -3.347160    -3.373651    -2.805707      24.34
 H      -4.125001    -2.655783    -0.062346      23.26
 H      -2.587282    -3.195543    -0.378356      24.21
 C       1.571142    -1.069640    -1.383820     -14.36
 H       2.109248    -1.497316    -2.299933      13.57
 C       1.488036     0.368720     0.634570     101.10
 H       1.743038     1.155147     1.440756      10.35
 C       0.109513     0.067536     0.835189      18.24
 O      -0.685031     0.567205     1.973118     186.62
 C      -0.056554     0.824714     3.335007      88.33
 H       1.042999     1.219710     3.182256      21.23
 H      -0.560035     2.023262     3.449150      19.98
 H      -0.661305     0.067107     4.032290      19.76
 C      -0.578816    -0.764912    -0.115220      14.72
 O      -1.990006    -0.927123     0.142498     199.86
 C       0.184964    -1.350452    -1.222608      27.48
 H      -0.262521    -1.858423    -2.031956      16.05
 C       2.181916    -0.272181    -0.481655      60.12
 C       3.773228    -0.000646    -0.697047      51.68
 H       4.234274    -0.210308    -1.796647      19.55
 O       4.214332     1.359832    -0.365419     246.38
 H       4.396006     1.349928     0.648867      24.09
 C       4.489726    -1.102579     0.121049     101.67
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 H       4.255854    -0.906417     1.236606      21.56
 O       3.902874    -2.397091    -0.122794     332.24
 H       4.113574    -2.486649    -1.038477      27.38
 C       6.134682    -1.302238    -0.274101      63.80
 O       7.108631    -0.239004     0.095099     289.82
 H       7.077726    -0.020421     1.055305      32.65
 H       6.101756    -1.494906    -1.384234      31.72
 H       6.154523    -2.436943     0.274934      27.89
55
name= lig-ACN-Water-frame_760
 C      -3.675903     1.376003    -2.946839      43.89
 H      -3.321079     0.437632    -3.577965      19.71
 C      -3.780530     2.368749    -0.578527      55.68
 H      -3.604855     2.356831     0.647683      17.78
 C      -3.669809     3.643983    -1.094480      10.43
 O      -3.471886     4.874007    -0.566211     180.43
 C      -4.137132     5.083981     0.870883      81.12
 H      -3.833012     6.292162     0.950607      23.89
 H      -3.702380     4.469709     1.552472      25.91
 H      -5.403303     5.255858     0.626650      22.48
 C      -3.660752     3.866892    -2.576466       2.99
 O      -3.413837     5.158888    -3.090388     144.13
 H      -3.849775     5.795654    -2.553928      26.01
 C      -3.417871     2.714846    -3.369480      51.59
 H      -3.149948     2.907114    -4.350428      24.18
 C      -4.034175     1.290057    -1.469474      16.78
 C      -4.126390    -0.175388    -0.978385      85.58
 H      -4.806060    -0.599462    -1.871572      23.23
 O      -4.818672    -0.463363     0.292418     205.00
 H      -4.405737     0.033139     1.002873      25.80
 C      -2.880533    -1.106557    -1.134617      59.09
 H      -2.344175    -0.865697    -1.989258      22.56
 C      -3.341731    -2.605316    -0.863350      89.67
 O      -4.100865    -3.375561    -2.074220     209.93
 H      -3.319357    -3.793043    -2.728270      23.73
 H      -4.161337    -2.462733    -0.213387      21.93
 H      -2.497506    -3.323796    -0.605224      21.57
 C       1.517455    -1.142214    -1.248554      70.90
 H       2.046846    -1.568041    -2.175110      14.48
 C       1.536373     0.324025     0.626705      63.52
 H       2.192331     0.935773     1.304934      11.96
 C       0.159478     0.103126     0.768393      -4.32
 O      -0.699043     0.579458     2.048966     146.80
 C      -0.041201     0.947779     3.309428      96.49
 H       1.134097     0.716590     3.388946      18.97
 H      -0.512329     1.927953     3.971040      20.94
 H      -0.017948    -0.004670     4.109675      22.52
 C      -0.535796    -0.711083    -0.153991      13.45
 O      -1.908057    -0.827552     0.098450     147.74
 C       0.121901    -1.235844    -1.250217     121.01
 H      -0.325711    -1.866641    -1.883232      20.36
 C       2.250652    -0.141458    -0.455434      35.25
 C       3.673231     0.059066    -0.670654      67.62
 H       3.751781    -0.093115    -1.864843      17.30
 O       4.155497     1.373259    -0.328374     275.10
 H       4.267554     1.506883     0.675621      24.44
 C       4.516450    -1.024335     0.127127      59.42
 H       4.329651    -0.902717     1.288512      22.80
 O       4.118679    -2.428223    -0.136395     329.00
 H       3.965940    -2.650389    -1.127602      25.91
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 C       6.130304    -1.284749    -0.185891      91.82
 O       7.006841    -0.314432     0.115023     279.48
 H       7.029106    -0.174719     1.062329      34.25
 H       6.263775    -1.303971    -1.280696      28.89
 H       6.670404    -2.331238     0.293120      26.04
55
name= lig-ACN-Water-frame_761
 C      -3.713995     1.496902    -2.744749      51.04
 H      -3.599030     0.586490    -3.358209      21.33
 C      -3.798945     2.414284    -0.582806      57.98
 H      -3.752919     2.237202     0.652118      16.59
 C      -3.601077     3.663489    -1.171343      38.77
 O      -3.505425     4.854572    -0.469950     256.47
 C      -4.053660     5.076596     0.739854      97.65
 H      -3.696090     6.138114     1.152106      24.94
 H      -3.791445     4.395952     1.518559      27.89
 H      -5.342534     4.719573     0.854492      23.00
 C      -3.557321     3.807803    -2.520714      22.10
 O      -3.373575     5.049184    -3.037299     161.14
 H      -3.695802     5.832471    -2.460493      24.50
 C      -3.408604     2.744815    -3.348258      66.76
 H      -3.102761     2.944876    -4.252570      26.80
 C      -3.935095     1.261362    -1.403573      40.04
 C      -4.200723    -0.223342    -0.989041      88.09
 H      -4.979004    -0.733161    -1.760172      24.32
 O      -4.895389    -0.523362     0.199920     219.49
 H      -4.569844     0.094127     0.924402      26.63
 C      -2.903260    -1.151280    -1.154385      68.10
 H      -2.420619    -1.059078    -2.162717      21.12
 C      -3.345160    -2.653779    -0.951554     110.77
 O      -4.069524    -3.331359    -2.045678     331.50
 H      -3.477242    -3.601029    -2.781129      28.77
 H      -3.867355    -2.817021    -0.104233      25.53
 H      -2.367853    -3.181481    -0.665686      23.36
 C       1.521863    -1.077645    -1.289986     -30.26
 H       2.091060    -1.778394    -1.941322      11.83
 C       1.557621     0.395313     0.735756      95.07
 H       2.084331     0.946726     1.469768      15.56
 C       0.125049     0.164359     0.963958      18.10
 O      -0.603563     0.578739     2.006163     223.65
 C       0.062226     0.870741     3.269732     107.04
 H       1.069295     1.467710     2.917913      19.18
 H      -0.496889     1.972171     3.646926      21.71
 H      -0.373506     0.112920     4.023558      21.84
 C      -0.600467    -0.554900    -0.129245      18.84
 O      -1.948711    -0.734673    -0.020261     167.23
 C       0.101279    -1.223103    -1.218163      48.16
 H      -0.410348    -1.846151    -1.842465      14.56
 C       2.180264    -0.206484    -0.454589      39.29
 C       3.725042     0.033850    -0.653976      64.57
 H       4.003105     0.082850    -1.799313      16.89
 O       4.096984     1.434946    -0.349759     281.40
 H       4.069371     1.480786     0.661603      22.62
 C       4.657123    -1.135692     0.092776      99.99
 H       4.541817    -0.789298     1.222099      20.33
 O       4.215693    -2.470660    -0.131250     235.57
 H       4.343686    -2.428159    -1.218958      19.43
 C       6.019065    -1.290861    -0.216248      78.19
 O       7.046894    -0.184574     0.193192     248.39
 H       7.228856    -0.247695     1.198551      31.36
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 H       6.102658    -1.605601    -1.244912      33.87
 H       6.140328    -2.336116     0.473876      26.62
55
name= lig-ACN-Water-frame_762
 C      -3.707301     1.462778    -2.691539      43.62
 H      -4.076627     0.803818    -3.397064      23.48
 C      -3.847246     2.364668    -0.484324      56.34
 H      -4.151879     2.307433     0.693667      19.00
 C      -3.611817     3.650715    -1.079964       7.43
 O      -3.452740     4.899901    -0.469253     195.16
 C      -4.050966     4.987125     0.891141     101.46
 H      -4.024391     6.106719     1.132427      23.46
 H      -3.445012     4.347215     1.567450      22.33
 H      -5.341121     4.927843     0.642967      22.59
 C      -3.366423     3.834809    -2.502034       1.61
 O      -3.339879     5.083577    -3.093508     153.04
 H      -3.129398     5.708399    -2.273825      23.10
 C      -3.474681     2.692524    -3.386546      39.15
 H      -3.608692     2.581216    -4.367684      24.40
 C      -3.827335     1.208371    -1.315660      34.69
 C      -4.207233    -0.294436    -1.113240      66.79
 H      -4.929934    -0.584289    -2.030094      22.24
 O      -4.988965    -0.494185     0.203167     162.99
 H      -4.314354    -0.201315     0.934829      24.51
 C      -2.964742    -1.186117    -1.110002      88.35
 H      -2.497108    -1.010547    -2.154649      21.36
 C      -3.221170    -2.759706    -0.967631     119.91
 O      -4.037350    -3.235598    -2.014114     333.61
 H      -3.616938    -3.134340    -2.817965      32.52
 H      -3.773190    -2.868804    -0.151416      25.91
 H      -2.221139    -3.320809    -1.056892      21.97
 C       1.483876    -1.011055    -1.345439      49.05
 H       1.966709    -1.548702    -2.158268      19.06
 C       1.491001     0.394441     0.772045      61.53
 H       1.978232     0.997993     1.443522      19.34
 C       0.155975     0.120886     0.903676      23.44
 O      -0.571476     0.574023     1.997624     209.56
 C       0.073368     0.975084     3.177609     116.78
 H       1.302709     1.096991     3.355418      20.83
 H      -0.705141     1.837663     3.589371      21.83
 H       0.325330     0.077097     3.933973      24.04
 C      -0.576157    -0.454622    -0.153055       8.73
 O      -2.130515    -0.640920    -0.099070     163.63
 C       0.109550    -1.176890    -1.079841      65.73
 H      -0.432608    -1.761621    -1.824497      18.30
 C       2.212802    -0.252848    -0.356455      13.18
 C       3.799352    -0.027134    -0.656492      67.11
 H       4.001660    -0.351397    -1.733971      21.41
 O       4.038338     1.451070    -0.357095     242.98
 H       4.403637     1.545689     0.594847      21.91
 C       4.581307    -1.064844     0.122030      85.84
 H       4.458844    -1.152180     1.300205      19.83
 O       4.177527    -2.512190    -0.136103     236.66
 H       4.027022    -2.857929    -1.157512      24.23
 C       6.271133    -1.211286    -0.189748      87.99
 O       7.031555    -0.143534     0.161611     271.08
 H       6.957737     0.023610     1.188279      28.25
 H       6.536838    -1.332290    -1.217704      29.66
 H       6.713935    -2.170126     0.448181      27.25
55
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name= lig-ACN-Water-frame_763
 C      -3.747745     1.354591    -2.785766      49.00
 H      -3.919226     0.504666    -3.279344      23.36
 C      -3.867590     2.355117    -0.414619      47.39
 H      -4.220191     2.315992     0.676630      18.44
 C      -3.547028     3.614224    -1.067468     -14.69
 O      -3.409113     4.913186    -0.424326     145.69
 C      -4.076099     4.993771     1.007458      95.14
 H      -3.930499     5.992660     1.316953      25.30
 H      -3.565890     4.290638     1.802838      22.78
 H      -5.240847     4.381551     1.129947      22.95
 C      -3.278109     3.758666    -2.515275      -7.34
 O      -3.242125     5.146092    -3.149443     143.17
 H      -3.233550     5.913229    -2.547472      25.20
 C      -3.565445     2.643637    -3.306154      43.08
 H      -3.728640     2.995471    -4.297790      21.54
 C      -3.821679     1.175904    -1.328805       1.59
 C      -4.266835    -0.300342    -1.034727      76.77
 H      -5.011784    -0.647804    -1.874890      22.45
 O      -5.010008    -0.441845     0.144356     203.69
 H      -4.353330    -0.457163     0.863384      25.81
 C      -2.951991    -1.239759    -1.152783      68.03
 H      -2.409357    -1.038454    -2.190133      20.13
 C      -3.052009    -2.757758    -0.921150     117.61
 O      -4.076990    -3.152725    -2.043079     278.69
 H      -3.551990    -3.175169    -2.972465      27.02
 H      -3.405542    -3.100834    -0.037476      26.53
 H      -2.079366    -3.321553    -0.948825      24.09
 C       1.487649    -0.931139    -1.254469       8.74
 H       1.853716    -1.134429    -2.244896      17.95
 C       1.581237     0.282874     0.672048      51.68
 H       2.117632     0.902758     1.344128      15.05
 C       0.080441     0.137866     0.831629      29.91
 O      -0.603316     0.574272     1.988960     180.62
 C       0.132070     1.039712     3.229037      83.24
 H       0.968116     1.746040     2.637004      18.59
 H      -0.408452     1.756990     4.014171      22.87
 H       0.108961     0.037452     3.765421      22.66
 C      -0.798652    -0.532913    -0.166481      22.43
 O      -2.119358    -0.500300    -0.038291     161.57
 C       0.083421    -1.150022    -1.146582      64.98
 H      -0.473309    -1.787405    -1.963807      13.20
 C       2.314549    -0.248519    -0.353587      32.93
 C       3.703445    -0.065428    -0.582545      75.41
 H       3.806536     0.016584    -1.674331      18.79
 O       4.044767     1.369791    -0.391587     261.32
 H       4.406960     1.490564     0.533159      23.13
 C       4.726730    -1.208737     0.159402      75.42
 H       4.486611    -0.772239     1.243250      20.15
 O       4.079009    -2.502852    -0.097143     325.73
 H       4.065445    -2.351390    -1.138094      22.79
 C       6.336581    -1.193291    -0.180671      77.36
 O       7.082843     0.040204     0.164884     308.96
 H       6.952681     0.294582     1.126669      32.11
 H       6.281569    -1.270096    -1.241915      32.00
 H       6.691928    -2.237012     0.235757      26.93
55
name= lig-ACN-Water-frame_764
 C      -3.771789     1.317076    -2.773148      56.60
 H      -3.644447     0.634910    -3.505581      23.39
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 C      -3.820299     2.330354    -0.591800      56.44
 H      -3.906179     2.141615     0.441963      18.02
 C      -3.425165     3.667567    -1.035284      13.72
 O      -3.472327     4.821723    -0.237524     231.11
 C      -3.994676     4.918880     1.033517     101.65
 H      -4.142677     5.902205     1.243520      25.65
 H      -3.199911     4.406255     1.803549      23.15
 H      -5.248926     4.592954     0.896318      23.96
 C      -3.356239     3.834213    -2.445824      28.93
 O      -3.122498     5.011419    -3.149422     217.94
 H      -3.674548     5.579154    -2.658897      24.37
 C      -3.617520     2.686886    -3.297078      34.21
 H      -3.481411     2.682322    -4.435895      20.69
 C      -3.947705     1.200038    -1.411810      29.78
 C      -4.235565    -0.301555    -1.021788      84.47
 H      -4.936404    -0.684455    -1.831127      22.57
 O      -5.037073    -0.425753     0.176862     211.42
 H      -4.587732    -0.286016     1.040616      23.82
 C      -2.921760    -1.152813    -1.051137      72.75
 H      -2.414942    -0.945059    -2.143307      17.85
 C      -3.026312    -2.737395    -0.997286     114.79
 O      -4.024183    -3.079974    -1.992258     313.90
 H      -3.429312    -3.588746    -2.764728      24.71
 H      -3.401720    -2.983077    -0.048039      23.62
 H      -2.051120    -3.109505    -1.320146      20.87
 C       1.416648    -0.941233    -1.331817      29.62
 H       1.924395    -1.424732    -2.176951      13.92
 C       1.448108     0.233763     0.769881     115.41
 H       1.954425     0.693160     1.648158      11.06
 C       0.089697     0.178711     0.837848      19.84
 O      -0.682944     0.628844     1.986305     193.87
 C       0.147681     1.070111     3.146793     102.19
 H       1.172054     1.798705     3.059585      18.64
 H      -0.734152     1.567964     3.558475      21.14
 H       0.928379     0.449897     3.743729      21.05
 C      -0.648030    -0.591977    -0.124023      38.38
 O      -2.127247    -0.458507    -0.005917     162.71
 C      -0.022333    -1.090788    -1.258616     149.66
 H      -0.279560    -1.682033    -2.275481      12.71
 C       2.181133    -0.316420    -0.366758      48.99
 C       3.829069    -0.067078    -0.620321      46.80
 H       4.076305    -0.452422    -1.591910      19.50
 O       4.121783     1.298891    -0.365838     286.68
 H       4.079216     1.453512     0.598969      22.32
 C       4.773585    -1.190800     0.199346      71.01
 H       4.870885    -1.275418     1.394236      18.32
 O       4.052292    -2.411585    -0.061047     355.44
 H       4.145750    -2.807715    -0.919974      30.16
 C       6.201139    -1.145750    -0.256800     119.84
 O       7.063401     0.120282     0.176167     251.11
 H       7.163116     0.196884     1.132044      32.34
 H       6.450293    -1.155898    -1.309288      32.87
 H       6.746807    -1.961408     0.199682      29.46
55
name= lig-ACN-Water-frame_765
 C      -3.772586     1.465312    -2.893381      55.25
 H      -3.900637     0.593017    -3.494405      22.20
 C      -3.738098     2.317965    -0.653817      54.37
 H      -3.777400     2.210463     0.330764      21.48
 C      -3.474895     3.621050    -1.024980      34.00
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 O      -3.424448     4.739788    -0.226652     230.96
 C      -3.995833     4.851739     1.119389     105.39
 H      -4.022408     5.843906     1.252563      27.38
 H      -3.367145     4.369448     2.058736      24.48
 H      -5.042493     4.145400     1.361107      24.76
 C      -3.475053     3.780371    -2.460243      36.37
 O      -3.050660     4.922419    -3.096125     105.76
 H      -3.283724     5.881479    -2.831695      19.84
 C      -3.552623     2.694914    -3.282277      49.97
 H      -3.296971     2.939084    -4.447817      20.65
 C      -4.052531     1.157727    -1.489379      16.47
 C      -4.223798    -0.268284    -1.002876      88.42
 H      -4.728398    -0.834640    -1.792011      20.68
 O      -5.090904    -0.419796     0.261626     233.78
 H      -4.434715     0.016262     0.923925      22.48
 C      -2.883292    -1.001034    -0.961235      63.22
 H      -2.450953    -0.625229    -2.060619      16.26
 C      -3.018418    -2.604044    -1.029535     120.63
 O      -3.967427    -3.052776    -1.976873     362.37
 H      -3.673707    -3.664024    -2.631697      29.58
 H      -3.216889    -3.045397    -0.055380      24.57
 H      -2.052942    -3.068836    -1.153320      25.43
 C       1.367604    -1.002149    -1.456667      40.59
 H       1.886002    -1.635836    -2.241495      18.28
 C       1.459859     0.186987     0.834823      77.09
 H       2.131765     0.576245     1.691684      14.95
 C       0.013834     0.112470     0.929135      10.01
 O      -0.642882     0.672984     1.948993     210.20
 C       0.095678     1.174767     3.060378      82.18
 H       0.515360     2.237489     2.570714      18.23
 H      -0.394221     1.350964     3.977707      23.57
 H       0.481146     0.048329     3.230553      18.43
 C      -0.656559    -0.544386    -0.167941      24.15
 O      -2.016324    -0.526005     0.025800     218.81
 C      -0.003026    -1.043810    -1.353233      57.39
 H      -0.970761    -1.417342    -1.895821       6.34
 C       2.125825    -0.326065    -0.317359      92.85
 C       3.832792    -0.166131    -0.510496      70.25
 H       4.015189    -0.150658    -1.551537      20.76
 O       4.218529     1.250026    -0.330456     255.58
 H       4.113028     1.487589     0.625773      23.58
 C       4.675179    -1.077459     0.213642      87.30
 H       4.602107    -0.803892     1.378639      19.57
 O       4.082608    -2.426519    -0.019407     342.28
 H       4.254311    -2.505708    -0.967840      26.00
 C       6.264333    -1.010216    -0.307503      94.20
 O       6.935231     0.032195     0.147991     347.94
 H       6.719454     0.227629     1.099517      36.18
 H       6.180685    -0.999892    -1.415684      30.63
 H       6.618888    -1.987469    -0.032637      27.82
55
name= lig-ACN-Water-frame_766
 C      -3.907820     1.374983    -2.938945      70.66
 H      -4.086176     0.653373    -3.789409      21.34
 C      -3.752428     2.184437    -0.527066      53.42
 H      -3.801309     1.971596     0.430414      21.08
 C      -3.655262     3.538534    -1.078762       5.20
 O      -3.333734     4.673959    -0.240334     155.88
 C      -3.982786     4.736273     1.237487      90.25
 H      -4.283202     5.687770     1.429494      25.98
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 H      -2.993107     4.401928     1.822251      21.38
 H      -5.093884     4.166573     1.144727      24.15
 C      -3.471551     3.828687    -2.455254      10.34
 O      -2.978534     4.984061    -3.083476     145.14
 H      -3.033438     5.624319    -2.241366      21.48
 C      -3.448657     2.747395    -3.416602      28.00
 H      -3.301112     3.204247    -4.594538      21.35
 C      -4.030030     1.247139    -1.539667      19.79
 C      -4.323367    -0.235153    -0.936312      92.71
 H      -4.946541    -0.795430    -1.576280      23.12
 O      -5.031122    -0.357119     0.267711     241.90
 H      -4.671507    -0.058025     1.154438      24.40
 C      -2.883569    -0.958294    -1.015791      57.01
 H      -2.336012    -0.652850    -2.089211      19.57
 C      -2.922861    -2.472811    -0.951758     111.23
 O      -3.978677    -3.019095    -1.988079     305.78
 H      -3.386424    -3.302705    -2.670615      27.19
 H      -3.370855    -2.687392     0.037750      23.05
 H      -1.965535    -2.821374    -1.238948      20.21
 C       1.422227    -0.980326    -1.377911      81.35
 H       1.942675    -1.218844    -2.394539      12.62
 C       1.511584     0.077467     0.778273      61.92
 H       2.134952     0.677274     1.542820      13.98
 C       0.145963     0.024818     0.921139      12.13
 O      -0.792092     0.720409     1.895088     172.67
 C       0.063834     1.188091     3.004192     124.01
 H       0.697974     2.298275     2.817849      22.11
 H      -0.656500     1.336034     3.673046      24.93
 H       1.185422     0.984402     3.325967      21.42
 C      -0.641175    -0.416787    -0.166617      25.80
 O      -1.975403    -0.603194     0.130971     152.34
 C      -0.061018    -0.986279    -1.305726     200.42
 H      -0.256459    -1.511684    -2.286235      19.77
 C       2.162324    -0.411846    -0.402242      37.46
 C       3.571566    -0.064860    -0.526845      81.22
 H       3.731999    -0.323395    -1.537812      22.00
 O       4.280048     1.217588    -0.259614     195.75
 H       4.400830     1.420694     0.718157      23.86
 C       4.655355    -1.092537     0.230233      68.53
 H       4.630496    -0.799319     1.375015      21.85
 O       4.194389    -2.445347     0.021763     252.85
 H       3.867749    -2.547264    -0.958015      26.69
 C       6.050711    -1.085140    -0.365249      91.41
 O       6.906350     0.086437     0.176131     256.72
 H       6.628950     0.309694     1.146871      31.55
 H       6.001770    -0.806668    -1.446166      27.69
 H       6.600988    -1.993213    -0.238794      28.80
55
name= lig-ACN-Water-frame_767
 C      -3.980079     1.508781    -2.975536      42.75
 H      -4.199034     0.575037    -3.612847      20.65
 C      -3.864839     2.223598    -0.591859      49.36
 H      -3.771498     2.018018     0.450834      18.82
 C      -3.698854     3.543430    -1.002738     -12.55
 O      -3.342047     4.613916    -0.181438     206.00
 C      -3.887874     4.614705     1.112629     132.22
 H      -4.210755     5.632049     1.321462      25.97
 H      -3.216991     4.319890     1.997102      25.52
 H      -4.657806     3.720974     1.273290      26.17
 C      -3.354272     3.746459    -2.565665       1.16
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 O      -2.950109     5.090572    -2.925684     144.18
 H      -2.953104     5.770487    -2.268751      25.45
 C      -3.523738     2.677069    -3.436007      62.83
 H      -3.269930     2.553651    -4.663688      21.00
 C      -4.047962     1.152140    -1.537295      19.29
 C      -4.285942    -0.183517    -1.012304      99.46
 H      -4.897607    -0.620793    -1.707680      24.32
 O      -4.996435    -0.288509     0.323810     230.34
 H      -4.288227     0.046426     0.886926      26.64
 C      -2.921897    -0.931201    -1.039340      61.36
 H      -2.352787    -0.435393    -2.016467      19.72
 C      -2.993032    -2.434182    -0.973164     113.21
 O      -3.869547    -2.960314    -1.926349     345.99
 H      -3.551516    -2.980754    -2.947024      28.50
 H      -3.307851    -2.790384     0.092272      23.91
 H      -2.044413    -2.959507    -0.956372      26.52
 C       1.400074    -0.897931    -1.394772       8.26
 H       1.864708    -1.188189    -2.426203      17.57
 C       1.542216     0.052437     0.831232      80.16
 H       2.187055     0.602416     1.556830      17.29
 C       0.095841     0.088328     0.884436      18.65
 O      -0.659790     0.665278     1.829351     187.91
 C       0.006938     1.386071     2.996142      92.76
 H      -0.147749     2.515427     2.599685      19.72
 H      -0.498681     1.254103     3.859248      25.87
 H       0.761048     0.492466     3.187280      20.82
 C      -0.648595    -0.489916    -0.191414      20.18
 O      -2.055481    -0.614107     0.173710     163.05
 C       0.073225    -0.988573    -1.308977      57.35
 H      -0.637756    -1.336628    -1.994104      12.06
 C       2.189284    -0.353496    -0.316484      60.09
 C       3.702750    -0.094742    -0.592759      80.73
 H       3.911326    -0.102495    -1.640367      24.37
 O       4.211666     1.238178    -0.208595     196.11
 H       4.363694     1.179229     0.755270      25.68
 C       4.524732    -1.151607     0.189664      91.71
 H       4.711937    -1.107534     1.317459      23.47
 O       4.240523    -2.540071     0.069919     247.81
 H       3.868214    -2.721712    -0.875642      26.35
 C       5.943177    -0.983891    -0.391559      94.23
 O       6.858012     0.121769     0.180051     232.15
 H       6.930701    -0.034638     1.157945      32.06
 H       5.940439    -0.925738    -1.507006      29.51
 H       6.366070    -1.858810    -0.135428      30.64
55
name= lig-ACN-Water-frame_768
 C      -4.057580     1.426607    -2.870657      57.26
 H      -4.217451     0.639025    -3.661009      25.17
 C      -3.973476     2.322499    -0.698184      57.32
 H      -4.030696     2.106004     0.446303      17.02
 C      -3.539831     3.548526    -1.191420      24.56
 O      -3.354579     4.555519    -0.241303     227.33
 C      -3.830674     4.490983     1.125984     121.93
 H      -4.356919     5.428010     1.260900      25.54
 H      -2.915848     4.457642     1.709537      25.89
 H      -4.761330     3.796636     1.255167      25.16
 C      -3.290264     3.811668    -2.440884      25.19
 O      -2.919856     5.063822    -2.813929     167.16
 H      -3.391899     5.660080    -2.222683      23.43
 C      -3.596357     2.721234    -3.423198      56.37
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 H      -3.270476     2.960823    -4.605590      18.54
 C      -4.144367     1.258917    -1.530001      38.95
 C      -4.272520    -0.238964    -1.060367     101.33
 H      -4.809130    -0.896657    -1.631391      25.34
 O      -4.917192    -0.205424     0.271508     262.13
 H      -4.411884    -0.060215     1.080069      23.07
 C      -2.904166    -0.922389    -0.972954      64.45
 H      -2.343781    -0.706416    -2.036287      19.43
 C      -3.004908    -2.482122    -0.924049     102.31
 O      -3.874732    -2.966166    -1.962066     318.69
 H      -3.257156    -2.945827    -2.817597      26.63
 H      -3.697209    -2.685191     0.010628      21.53
 H      -1.977855    -2.831008    -1.041346      22.15
 C       1.513475    -0.795890    -1.454772      35.88
 H       2.100428    -1.306474    -2.292322      17.48
 C       1.511950     0.137323     0.913619      70.42
 H       1.968536     0.458515     1.819888      16.64
 C       0.154900     0.142935     0.820174      15.77
 O      -0.606278     0.645788     1.911672     219.18
 C      -0.126059     1.449687     2.932411     125.91
 H       0.203624     2.597455     2.790626      21.22
 H      -0.840254     1.317248     3.682213      23.35
 H       1.100478     1.473300     3.204587      19.08
 C      -0.710748    -0.601577    -0.085002       8.29
 O      -2.068101    -0.561592     0.080070     183.84
 C      -0.060864    -1.016625    -1.299549      90.76
 H      -0.417418    -1.458519    -2.106175      20.18
 C       2.230597    -0.271641    -0.381145      25.15
 C       3.755860    -0.153073    -0.572687      82.59
 H       3.946416    -0.248441    -1.656464      22.75
 O       4.079027     1.244310    -0.167648     223.91
 H       4.316548     1.461773     0.755200      24.49
 C       4.573094    -1.163985     0.176595      81.77
 H       4.208702    -0.770153     1.141197      23.67
 O       4.175013    -2.677701     0.060680     286.62
 H       4.217130    -2.809762    -0.885659      29.40
 C       6.064894    -0.932520    -0.336753     111.60
 O       6.765317     0.101136     0.153609     313.55
 H       7.104891    -0.148928     1.013264      33.68
 H       5.995478    -0.711500    -1.412447      31.52
 H       6.580246    -1.801523    -0.221596      28.65
55
name= lig-ACN-Water-frame_769
 C      -4.037135     1.495099    -3.012730      35.41
 H      -4.211141     0.672477    -3.707602      21.65
 C      -4.060105     2.310100    -0.679921      56.25
 H      -4.424998     2.260298     0.492475      16.78
 C      -3.447641     3.492157    -1.080896      26.54
 O      -3.341289     4.618140    -0.336402     205.54
 C      -3.819038     4.443199     1.142993     129.79
 H      -4.277624     5.445116     1.475681      25.16
 H      -2.987901     4.325831     1.776824      30.95
 H      -4.317993     3.559256     1.366019      27.81
 C      -3.292283     3.781059    -2.524499      18.22
 O      -2.861180     5.073500    -2.807147      68.22
 H      -3.387486     5.912136    -2.420895      17.36
 C      -3.645715     2.790816    -3.333321      49.14
 H      -3.760032     3.084187    -4.487026      22.64
 C      -4.266506     1.200843    -1.579663      21.04
 C      -4.256429    -0.192645    -0.966479     114.67
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 H      -4.868881    -0.678551    -1.647855      23.17
 O      -4.937655    -0.196957     0.223171     272.85
 H      -4.259103     0.065914     0.905413      23.92
 C      -2.876331    -1.024513    -1.048964      69.07
 H      -2.366061    -0.755302    -2.073327      19.66
 C      -3.067602    -2.494362    -0.830990      94.57
 O      -3.894282    -3.003891    -2.077618     322.64
 H      -3.384006    -3.478771    -2.713546      28.68
 H      -3.469605    -2.853612     0.261633      22.48
 H      -2.153258    -3.152454    -0.760008      23.14
 C       1.348608    -0.765378    -1.369597      28.47
 H       1.812512    -1.032151    -2.321540      20.86
 C       1.580364     0.185593     0.743007      60.32
 H       2.138861     0.547495     1.539261      18.47
 C       0.110386     0.112136     0.900191       9.25
 O      -0.641782     0.604773     1.970368     180.25
 C      -0.105180     1.646835     2.936834      94.47
 H      -0.545497     2.524939     2.371118      19.06
 H      -0.824361     1.565966     3.761981      22.34
 H       0.781121     1.233404     3.616280      20.81
 C      -0.611474    -0.589529    -0.135004      14.08
 O      -2.035533    -0.440464     0.075978     144.76
 C       0.086340    -1.038820    -1.308930      65.40
 H      -0.390083    -1.578292    -1.968839      18.33
 C       2.183549    -0.222330    -0.372916      46.95
 C       3.629617    -0.116187    -0.542880      62.03
 H       3.926286    -0.185736    -1.637719      20.51
 O       3.983778     1.263472    -0.194379     188.16
 H       4.180454     1.205304     0.783843      21.62
 C       4.657270    -1.249078     0.249346      85.04
 H       4.927295    -1.360673     1.286844      22.64
 O       4.136824    -2.628992     0.009973     303.65
 H       4.297344    -2.937899    -0.904573      27.48
 C       6.127299    -1.120798    -0.340670      96.64
 O       6.766753     0.198986     0.213393     271.18
 H       7.075556     0.221620     1.196324      29.26
 H       5.974309    -0.882070    -1.379224      30.40
 H       6.693945    -1.927046    -0.342695      30.85
55
name= lig-ACN-Water-frame_770
 C      -4.042880     1.517883    -3.025563      37.45
 H      -4.150288     0.810988    -3.819126      23.18
 C      -4.113442     2.216116    -0.700423      60.17
 H      -4.513731     1.822318     0.400447      15.42
 C      -3.508074     3.476445    -1.027303      17.72
 O      -3.367393     4.713067    -0.210725     235.61
 C      -3.676402     4.463074     1.100801     155.95
 H      -4.325537     5.425280     1.390774      24.43
 H      -2.829193     4.335985     1.661448      29.40
 H      -4.413579     3.773133     1.166400      30.65
 C      -3.298544     3.814011    -2.394440      13.21
 O      -2.794868     5.075277    -2.911310      78.34
 H      -3.180119     5.796310    -2.199678      21.05
 C      -3.724700     2.829474    -3.486174      33.11
 H      -3.788327     3.059084    -4.588478      22.13
 C      -4.184624     1.226198    -1.652013      47.35
 C      -4.301004    -0.205500    -1.132320      72.15
 H      -4.908335    -0.930324    -1.631586      23.84
 O      -4.993004    -0.228435     0.304180     126.81
 H      -4.468795     0.138233     1.123179      19.96
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 C      -2.891754    -0.985068    -1.027680      62.60
 H      -2.451377    -0.905306    -2.073216      20.98
 C      -3.166125    -2.653245    -0.912077      99.90
 O      -3.886530    -3.017218    -2.035285     322.23
 H      -3.423997    -3.758487    -2.445903      27.05
 H      -4.003529    -2.657494    -0.076663      20.97
 H      -2.083280    -3.027801    -0.809766      20.59
 C       1.458963    -0.823571    -1.487018      43.98
 H       1.910198    -1.028807    -2.425198      23.12
 C       1.461946     0.286343     0.807136      72.72
 H       2.085050     0.896455     1.389075      18.74
 C       0.155920     0.083770     0.984086      20.46
 O      -0.653273     0.527069     2.038239     197.62
 C      -0.225775     1.748207     2.896313     100.13
 H       0.073546     2.775665     2.506050      22.72
 H      -0.880378     1.763935     3.874746      22.31
 H       0.891239     1.649593     2.909702      21.60
 C      -0.614591    -0.434623    -0.112390      13.25
 O      -1.965979    -0.400446     0.002001     139.86
 C      -0.057311    -1.092583    -1.214701      81.39
 H      -0.592123    -1.490670    -2.046546      19.34
 C       2.121627    -0.268261    -0.395248      15.53
 C       3.696485    -0.103099    -0.448269      56.56
 H       3.903067    -0.340437    -1.562412      21.06
 O       3.956255     1.286600    -0.202993     217.97
 H       4.192075     1.555009     0.730348      23.22
 C       4.749445    -1.350727     0.250049      74.41
 H       4.577096    -1.076014     1.278986      23.31
 O       4.123524    -2.545169    -0.046691     294.08
 H       4.139478    -2.604562    -1.115979      23.96
 C       6.180078    -1.126263    -0.320268     110.62
 O       6.742657     0.188168     0.215881     327.95
 H       6.544814     0.146377     1.203486      31.18
 H       6.334038    -1.070130    -1.375645      29.45
 H       6.657675    -1.878985     0.091954      28.95
55
name= lig-ACN-Water-frame_771
 C      -4.037655     1.549405    -3.120574      60.40
 H      -4.244353     0.732162    -3.823651      22.36
 C      -4.046253     2.274521    -0.698744      47.72
 H      -4.156174     2.029446     0.468680      16.72
 C      -3.653621     3.604036    -1.062006      12.65
 O      -3.371336     4.653837    -0.245396     213.35
 C      -3.639954     4.537662     1.239409     123.64
 H      -3.911465     5.611817     1.724596      23.51
 H      -2.774040     4.277219     1.724452      29.78
 H      -4.304752     3.841295     1.419961      30.64
 C      -3.359172     3.814037    -2.502468      34.64
 O      -2.786597     4.962302    -2.930863     175.44
 H      -3.078766     5.737263    -2.388505      24.72
 C      -3.717711     2.925328    -3.440717      62.00
 H      -3.429110     3.235025    -4.388818      24.01
 C      -4.109215     1.187540    -1.705780       8.27
 C      -4.320277    -0.282080    -1.076880      80.54
 H      -4.980518    -0.795530    -1.827188      22.76
 O      -5.036407    -0.249804     0.257387     161.81
 H      -4.229305    -0.116059     0.862675      23.46
 C      -2.945511    -1.004020    -1.045062      84.85
 H      -2.483466    -0.823527    -2.010913      20.77
 C      -3.212586    -2.545765    -0.882726     103.35
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 O      -3.917121    -3.079938    -2.042973     311.92
 H      -3.380136    -3.592228    -2.879960      22.90
 H      -3.696986    -2.912379     0.160867      22.26
 H      -2.326595    -3.303841    -0.698468      20.47
 C       1.398638    -0.953962    -1.444458      45.28
 H       1.897791    -1.456512    -2.214338      22.53
 C       1.523425     0.334242     0.789292      53.66
 H       1.941846     0.926967     1.619231      17.17
 C       0.034757     0.140778     1.023774      -6.17
 O      -0.680240     0.576185     2.167694     207.61
 C      -0.152620     1.745514     2.741948      97.47
 H      -0.758016     2.539080     2.130985      19.25
 H      -0.813698     1.741429     3.765858      21.37
 H       0.800791     1.626244     3.248145      22.25
 C      -0.653143    -0.433951    -0.124361       4.85
 O      -2.091234    -0.392139    -0.062171     186.09
 C       0.041346    -1.030206    -1.247918      54.99
 H      -0.724155    -1.397184    -2.019341      16.57
 C       2.203241    -0.305169    -0.339905      17.69
 C       3.730631    -0.150703    -0.435216      83.36
 H       4.059421    -0.054800    -1.546542      20.08
 O       4.006665     1.357241    -0.199409     182.18
 H       4.129092     1.492315     0.772005      23.14
 C       4.643510    -1.132458     0.188859     100.16
 H       4.763583    -1.260333     1.279506      22.74
 O       4.132685    -2.524106    -0.138614     265.14
 H       3.877582    -2.666494    -1.156425      23.53
 C       6.217068    -1.075286    -0.178047      98.78
 O       6.685428     0.118312     0.192550     331.91
 H       6.591244     0.313526     1.117457      32.19
 H       6.262709    -1.191542    -1.255626      29.75
 H       6.779544    -2.034653     0.085774      28.30
55
name= lig-ACN-Water-frame_772
 C      -4.045577     1.538823    -3.072429      56.16
 H      -4.159985     0.898139    -4.008075      20.64
 C      -3.915569     2.320749    -0.782339      57.05
 H      -3.893995     2.149031     0.308787      22.10
 C      -3.775249     3.620648    -1.144061      26.08
 O      -3.384632     4.638506    -0.234020     166.36
 C      -3.576541     4.566582     1.367359      95.44
 H      -3.712640     5.772269     1.464275      21.60
 H      -2.655052     4.183846     1.680929      25.80
 H      -4.362285     4.122179     1.703758      28.47
 C      -3.480741     3.854615    -2.491412      27.50
 O      -2.756625     4.947265    -2.947348      93.87
 H      -3.204776     5.723139    -2.695646      26.52
 C      -3.667999     2.825729    -3.464924      45.98
 H      -3.525607     3.026820    -4.416915      23.47
 C      -4.110326     1.250596    -1.645247      34.48
 C      -4.324577    -0.212552    -1.086730      95.17
 H      -5.013816    -0.890569    -1.762551      22.85
 O      -4.989279    -0.242378     0.125083     231.88
 H      -4.506441    -0.117308     0.945195      25.50
 C      -3.021703    -1.078529    -1.128053      86.81
 H      -2.676178    -0.958131    -2.116202      23.85
 C      -3.145061    -2.564455    -0.849586      93.67
 O      -4.010934    -3.104700    -2.029291     278.19
 H      -3.177957    -3.132644    -2.686031      25.48
 H      -3.862502    -2.585170     0.018974      23.51
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 H      -1.996899    -2.865981    -0.807672      20.96
 C       1.481106    -1.048841    -1.149965      56.66
 H       1.862217    -1.631386    -1.955442      14.33
 C       1.454150     0.254978     0.748263      48.28
 H       2.267873     0.601485     1.459959      13.26
 C       0.011054     0.184679     0.898209      15.56
 O      -0.638442     0.495414     2.159718     221.98
 C      -0.201134     1.811376     2.732276      97.54
 H      -0.303289     2.771369     1.914475      21.12
 H      -0.788114     2.115216     3.765337      21.03
 H       0.787067     2.004117     2.626930      23.68
 C      -0.734423    -0.479478    -0.127272      12.85
 O      -2.206799    -0.392138    -0.054708     155.38
 C       0.006426    -0.890227    -1.245990      68.99
 H      -0.314855    -1.601420    -2.176077      17.28
 C       2.188346    -0.315459    -0.278187      21.81
 C       3.715788     0.027432    -0.557317      53.10
 H       3.804804    -0.297262    -1.693187      17.83
 O       4.081021     1.366089    -0.164125     205.66
 H       3.991898     1.541753     0.822698      22.09
 C       4.606480    -1.160971     0.206983      79.50
 H       4.313844    -0.892105     1.293780      22.34
 O       4.140509    -2.462605    -0.196199     291.74
 H       4.243157    -2.498536    -1.224385      25.43
 C       6.038954    -1.142380    -0.196501      86.58
 O       6.748535     0.226941     0.228015     251.26
 H       6.883716     0.258890     1.211842      30.39
 H       6.180803    -1.041739    -1.262513      31.28
 H       6.416634    -2.079271     0.387283      27.98
55
name= lig-ACN-Water-frame_773
 C      -4.052282     1.480358    -2.980712      50.29
 H      -4.220289     0.477814    -3.569329      21.03
 C      -3.865984     2.275625    -0.713574      43.04
 H      -3.763002     2.000989     0.264446      22.21
 C      -3.745705     3.673016    -1.107400       1.01
 O      -3.455331     4.655660    -0.152281     206.25
 C      -3.476756     4.598900     1.252342     126.10
 H      -3.381083     5.682821     1.674589      24.35
 H      -2.698439     4.100441     1.806151      27.79
 H      -4.383169     4.246908     1.506971      28.36
 C      -3.542034     3.902463    -2.591291      -2.59
 O      -2.782854     5.022872    -2.976145      66.27
 H      -3.152432     5.828539    -2.515005      24.79
 C      -3.639993     2.757063    -3.489756      58.14
 H      -3.535148     2.902778    -4.445435      24.15
 C      -4.143443     1.228677    -1.683257      37.49
 C      -4.309183    -0.158979    -1.239943      84.57
 H      -5.080473    -0.577606    -2.067627      22.31
 O      -5.001933    -0.225106     0.120106     182.45
 H      -4.321380     0.199112     0.660900      26.75
 C      -3.022942    -0.997874    -1.188775      87.57
 H      -2.455455    -0.882079    -2.016412      24.34
 C      -3.202759    -2.547637    -0.926391     113.64
 O      -3.986924    -3.084406    -1.884987     370.01
 H      -3.762971    -3.418597    -2.699323      31.83
 H      -3.553650    -2.914732     0.067440      24.07
 H      -2.198489    -3.207809    -0.870503      21.91
 C       1.417552    -1.139230    -1.087668      39.78
 H       2.053417    -1.574992    -1.864964      16.92
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 C       1.413863     0.221491     0.850264      42.53
 H       1.549190     0.829439     1.814733      14.62
 C      -0.005127     0.161957     0.859284      12.79
 O      -0.564015     0.476290     2.090047     207.63
 C      -0.182606     1.933467     2.597655      77.92
 H      -0.743728     2.811664     1.917821      20.73
 H      -0.575270     1.932130     3.753275      22.57
 H       0.751083     1.828530     2.839315      24.27
 C      -0.851731    -0.401771    -0.167706      14.66
 O      -2.190748    -0.440882    -0.081921     191.45
 C       0.012575    -0.974207    -1.180582      58.74
 H      -0.637917    -1.412034    -2.130044      18.68
 C       2.211391    -0.247082    -0.243314      22.94
 C       3.630356     0.035118    -0.542357      84.07
 H       3.884804     0.298577    -1.669599      18.34
 O       4.138485     1.353967    -0.189206     202.34
 H       4.092599     1.567944     0.805905      23.81
 C       4.445850    -1.062806     0.152410      86.66
 H       4.265941    -1.139041     1.336204      22.61
 O       4.128135    -2.402286    -0.211783     310.16
 H       4.265885    -2.662306    -1.161994      28.70
 C       6.006789    -0.975540    -0.123601      92.09
 O       6.801220     0.205570     0.234683     279.08
 H       6.834254     0.260091     1.265038      28.82
 H       6.102458    -1.285055    -1.184794      29.12
 H       6.699113    -1.861552     0.358709      25.94
55
name= lig-ACN-Water-frame_774
 C      -4.030253     1.481557    -3.077524      46.21
 H      -4.215050     0.671653    -3.973989      19.94
 C      -3.884159     2.314917    -0.622428      68.88
 H      -3.839436     2.188898     0.337585      21.84
 C      -3.602648     3.576818    -1.099426      19.83
 O      -3.477149     4.745656    -0.256341     218.29
 C      -3.462953     4.545100     1.205164      98.65
 H      -3.220264     5.553135     1.597512      24.91
 H      -2.721927     3.758721     1.345888      27.67
 H      -4.317603     4.234684     1.600458      29.38
 C      -3.482079     3.850403    -2.516766      17.48
 O      -2.914063     5.080995    -3.009174      33.53
 H      -3.275563     5.883411    -2.376006      19.14
 C      -3.678734     2.793687    -3.483643      48.04
 H      -3.351422     2.972368    -4.444815      23.19
 C      -4.116056     1.285777    -1.544651       8.10
 C      -4.379418    -0.195748    -1.222897      78.84
 H      -5.037176    -0.907866    -1.976879      21.00
 O      -4.987423    -0.205370     0.051760     193.06
 H      -4.350288     0.021632     0.827146      22.59
 C      -2.921211    -0.977997    -1.208746      89.43
 H      -2.556285    -0.780485    -2.121585      26.07
 C      -3.121105    -2.519017    -0.939935     107.64
 O      -4.155538    -3.143309    -1.845029     317.92
 H      -3.525704    -3.713385    -2.270423      27.25
 H      -3.504569    -2.455751     0.053006      25.53
 H      -2.005449    -2.881928    -1.102249      21.26
 C       1.357430    -1.037037    -1.155386      46.88
 H       1.732897    -1.631046    -2.021170      19.85
 C       1.382573     0.257921     0.897316      64.67
 H       2.168310     0.788660     1.564405      15.65
 C      -0.043816     0.111130     0.937753      10.84
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 O      -0.574661     0.617673     2.072955     202.96
 C      -0.204318     1.870338     2.549470      93.83
 H      -0.633216     2.694115     1.654469      22.70
 H      -0.982270     1.950839     3.445292      22.00
 H       0.648329     2.333252     2.580763      25.72
 C      -0.729282    -0.349889    -0.251253       8.66
 O      -2.200801    -0.454072    -0.097187     172.88
 C      -0.023852    -1.183823    -1.126090      55.33
 H      -0.509834    -1.722505    -2.080660      19.18
 C       2.025880    -0.219374    -0.194536      18.20
 C       3.581612     0.050918    -0.490911      67.61
 H       3.597462    -0.373315    -1.599339      20.69
 O       4.148105     1.386445    -0.188023     202.27
 H       4.140613     1.574265     0.805272      23.65
 C       4.464807    -1.004722     0.141995      71.74
 H       4.258397    -0.805845     1.330266      21.48
 O       4.094282    -2.389065    -0.194257     295.83
 H       4.060292    -2.372714    -1.210491      24.66
 C       6.063756    -0.879062    -0.061568      73.28
 O       6.846225     0.219796     0.223984     323.00
 H       6.760733     0.630076     1.118341      30.60
 H       6.213998    -0.835115    -1.173626      26.50
 H       6.136896    -1.937713     0.544799      25.35
55
name= lig-ACN-Water-frame_775
 C      -3.992769     1.612044    -3.005873      47.84
 H      -4.195153     0.744950    -3.844239      22.67
 C      -3.922313     2.291528    -0.616244      41.19
 H      -4.218942     2.082569     0.333120      21.53
 C      -3.477151     3.627177    -1.104414      11.53
 O      -3.492426     4.772466    -0.396828     181.07
 C      -3.435749     4.443467     1.118730     125.95
 H      -2.932549     5.234666     1.524902      23.92
 H      -2.678188     3.615743     1.342670      22.55
 H      -4.343234     4.311378     1.552631      24.92
 C      -3.310781     3.814166    -2.463779      30.31
 O      -3.109234     5.051842    -3.009082     114.21
 H      -3.622601     5.810429    -2.397211      19.54
 C      -3.665913     2.881952    -3.432024      43.90
 H      -3.667525     3.213981    -4.512891      23.18
 C      -4.105952     1.242669    -1.667513       5.87
 C      -4.271472    -0.196769    -1.131632      77.44
 H      -5.056620    -0.690159    -1.928101      21.85
 O      -5.031223    -0.269660     0.097261     185.53
 H      -4.351740    -0.123699     0.826377      23.63
 C      -2.981082    -0.954753    -1.273685      80.73
 H      -2.456747    -0.744711    -2.117956      23.69
 C      -3.078892    -2.428980    -0.949469     108.44
 O      -4.224428    -3.197654    -1.774894     211.71
 H      -3.935392    -3.993194    -2.462955      23.93
 H      -3.279518    -2.596895     0.061429      25.68
 H      -2.219404    -3.177434    -1.079281      21.46
 C       1.321407    -0.945881    -1.276018      40.06
 H       2.107549    -1.275733    -1.999530      19.01
 C       1.420546     0.302038     0.857627      66.47
 H       1.870232     0.735106     1.790293      15.72
 C       0.035396     0.172225     1.007944       1.32
 O      -0.712966     0.636848     2.084728     238.32
 C      -0.339860     2.037094     2.486920      82.93
 H      -0.704531     2.836767     1.577494      19.56
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 H      -0.752838     2.338503     3.475453      23.96
 H       0.646120     1.821952     2.681084      22.93
 C      -0.771271    -0.474431    -0.140322      -7.24
 O      -2.094314    -0.406424    -0.115073     113.49
 C      -0.063129    -1.288374    -1.132245      62.89
 H      -0.535701    -2.110746    -1.752471      18.72
 C       2.035465    -0.248454    -0.327927      38.55
 C       3.497099     0.013907    -0.486169      75.63
 H       3.756651     0.230833    -1.604215      18.25
 O       4.062719     1.374700    -0.235711     186.69
 H       3.973726     1.658331     0.709379      23.71
 C       4.527921    -0.961838     0.267204      81.24
 H       4.363837    -1.013954     1.478068      20.35
 O       4.078039    -2.289084    -0.130872     302.62
 H       4.296662    -2.554476    -1.138680      24.30
 C       5.994517    -0.941249    -0.102421      99.08
 O       6.934985     0.361537     0.279122     257.81
 H       6.817910     0.520750     1.234464      30.67
 H       6.223113    -1.300771    -1.162877      27.93
 H       6.788040    -1.649990     0.448786      24.58
55
name= lig-ACN-Water-frame_776
 C      -3.979563     1.604822    -3.015540      40.76
 H      -4.236363     0.748041    -3.808215      21.59
 C      -3.936559     2.303148    -0.763070      89.40
 H      -4.258314     2.122689     0.280093      20.96
 C      -3.482652     3.517590    -1.104818       3.42
 O      -3.459807     4.704481    -0.309511     246.08
 C      -3.356982     4.444291     1.003839     127.82
 H      -2.939730     5.175689     1.510836      27.78
 H      -2.960645     3.344067     1.138777      23.26
 H      -4.346904     4.274616     1.289006      26.91
 C      -3.215370     3.837085    -2.508593      14.18
 O      -3.266649     5.121369    -3.029041     126.34
 H      -3.317146     5.844568    -2.260604      22.51
 C      -3.604397     2.888756    -3.418209      36.40
 H      -3.966278     3.249574    -4.507103      22.59
 C      -4.059086     1.289327    -1.581234      34.99
 C      -4.284442    -0.125872    -1.194867      64.78
 H      -4.917350    -0.754614    -2.008549      22.56
 O      -5.011832    -0.363873     0.198049     151.52
 H      -4.442435    -0.051790     0.907391      25.38
 C      -2.917167    -0.954531    -1.208681      70.90
 H      -2.576134    -0.768468    -2.194918      24.32
 C      -3.179719    -2.602176    -1.016126     111.50
 O      -4.225050    -3.167195    -1.628529     312.28
 H      -3.778276    -3.464484    -2.519068      25.90
 H      -3.361786    -2.638591    -0.011436      26.92
 H      -2.144127    -2.897635    -1.311206      22.56
 C       1.333647    -0.942348    -1.379333      54.45
 H       1.617381    -1.404823    -2.360694      17.55
 C       1.415156     0.284712     0.822957      40.52
 H       2.097478     0.717319     1.547719      14.19
 C      -0.065810     0.172643     0.903758       7.93
 O      -0.872266     0.644853     2.070047     110.32
 C      -0.387724     2.188069     2.481906      84.65
 H      -0.490187     3.009435     1.530306      20.41
 H      -1.074956     2.320027     3.259222      22.86
 H       0.669167     2.309806     2.687635      22.86
 C      -0.674177    -0.687890     0.012557      17.16
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 O      -2.097612    -0.365440    -0.130049     144.85
 C      -0.003850    -1.234569    -1.087697      61.55
 H      -0.582044    -1.858274    -1.679914      19.46
 C       2.111458    -0.157455    -0.346017      31.62
 C       3.662670     0.055828    -0.520049      68.62
 H       3.873074    -0.430355    -1.564014      22.14
 O       3.906237     1.428719    -0.244326     214.88
 H       3.951552     1.544468     0.741845      22.74
 C       4.497004    -0.972246     0.288692      79.45
 H       4.412223    -0.747802     1.477837      22.28
 O       4.071306    -2.265719    -0.041069     316.73
 H       4.495587    -2.498443    -0.942173      27.09
 C       6.186073    -0.841965    -0.051997      65.25
 O       6.896207     0.385038     0.243407     288.85
 H       6.962366     0.470495     1.258303      29.77
 H       6.103017    -0.855605    -1.183888      31.43
 H       6.420711    -1.870511     0.590025      28.23
55
name= lig-ACN-Water-frame_777
 C      -3.948981     1.501266    -3.046127      54.16
 H      -4.296413     0.816728    -3.882841      24.52
 C      -3.940388     2.350816    -0.666904      33.02
 H      -4.054870     2.246936     0.529457      16.08
 C      -3.461485     3.636201    -1.221710      16.01
 O      -3.361028     4.633087    -0.365804     190.19
 C      -3.393450     4.367745     1.157161      84.86
 H      -2.799005     5.112626     1.440289      25.36
 H      -2.659132     3.465415     1.445619      22.69
 H      -4.248635     4.432023     1.681110      25.31
 C      -3.322540     3.885118    -2.567941      17.28
 O      -3.287984     5.217387    -3.066094     153.96
 H      -3.543412     5.876248    -2.362496      24.03
 C      -3.588177     2.796191    -3.469216      38.00
 H      -3.476530     3.067747    -4.696558      19.31
 C      -4.061951     1.231190    -1.672613       4.30
 C      -4.311524    -0.230375    -1.090803      81.96
 H      -5.069379    -0.753393    -1.792251      23.03
 O      -4.932229    -0.407036     0.163322     218.35
 H      -4.290205    -0.194873     0.890096      24.38
 C      -2.933907    -1.010833    -1.134774      90.10
 H      -2.356286    -0.857701    -2.021948      24.78
 C      -3.067300    -2.542320    -0.895433     111.52
 O      -4.292599    -3.181642    -1.616699     318.19
 H      -4.262763    -3.217629    -2.504068      33.67
 H      -3.170606    -2.821148     0.083667      27.86
 H      -2.305230    -3.235566    -1.294427      23.44
 C       1.421510    -0.916342    -1.337476      24.69
 H       1.912906    -1.165138    -2.294910      19.05
 C       1.345430     0.252101     0.723326      71.00
 H       1.763229     0.869016     1.477758      17.50
 C      -0.036587     0.134427     1.000693       5.48
 O      -0.800064     0.823225     1.946977     214.96
 C      -0.478967     2.167832     2.436476     101.94
 H      -0.716634     2.831298     1.401776      19.81
 H      -1.251278     2.465478     3.039410      23.97
 H       0.441642     2.285723     3.012828      22.44
 C      -0.763679    -0.708781     0.036641      -5.33
 O      -2.101616    -0.424089    -0.135320     154.34
 C       0.037806    -1.206880    -1.078645      66.66
 H      -0.376190    -1.464144    -1.937823      22.33
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 C       2.094619    -0.202348    -0.437643      26.63
 C       3.683421     0.023940    -0.555993      77.28
 H       4.013737     0.113638    -1.648835      20.69
 O       3.825711     1.512103    -0.274554     182.42
 H       4.133993     1.687215     0.670252      22.25
 C       4.626387    -0.848499     0.328539      76.00
 H       4.254804    -0.740830     1.451998      21.30
 O       4.123489    -2.291534     0.063854     315.57
 H       4.169771    -2.471276    -0.896440      28.13
 C       6.131334    -0.776702    -0.002247     103.06
 O       6.855747     0.391463     0.241450     273.43
 H       6.856161     0.725494     1.242752      29.37
 H       6.419343    -0.982283    -1.092991      27.01
 H       6.874119    -1.723483     0.384292      24.85
55
name= lig-ACN-Water-frame_778
 C      -3.911467     1.432500    -3.025378      46.83
 H      -3.976878     0.577607    -3.677154      21.24
 C      -3.850613     2.299154    -0.821881      70.18
 H      -3.950254     2.025743     0.381912      17.49
 C      -3.574113     3.567721    -1.194667       2.07
 O      -3.263960     4.676794    -0.265077     174.54
 C      -3.293150     4.404388     1.253469      78.78
 H      -2.828942     5.248442     1.661449      25.45
 H      -2.837552     3.379645     1.523802      23.74
 H      -4.360162     4.247773     1.410109      25.07
 C      -3.539559     3.917225    -2.716560      -7.64
 O      -3.230045     5.229205    -3.129956      53.05
 H      -3.707950     5.837651    -2.594088      26.54
 C      -3.550948     2.786161    -3.541038      53.17
 H      -3.217302     2.902214    -4.725404      18.46
 C      -4.116077     1.212914    -1.594863      19.92
 C      -4.254960    -0.340046    -1.102179      86.22
 H      -4.883001    -0.899706    -1.830083      23.24
 O      -4.883060    -0.413291     0.196216     233.29
 H      -4.207674    -0.252195     0.980982      20.12
 C      -2.948525    -1.118286    -1.139317      76.77
 H      -2.667724    -0.915309    -2.203409      22.87
 C      -3.021733    -2.614057    -0.861788     109.53
 O      -4.360357    -3.148565    -1.518785     234.92
 H      -4.124275    -3.095606    -2.527371      27.06
 H      -3.234754    -2.763877     0.165926      25.48
 H      -2.067178    -2.979978    -1.160701      23.93
 C       1.422786    -0.981311    -1.344289      43.95
 H       1.941053    -1.323760    -2.248429      20.78
 C       1.365582     0.321675     0.747258      67.36
 H       1.904495     1.049564     1.317182      17.12
 C      -0.004531     0.048046     0.967226      12.35
 O      -0.714922     0.884774     1.808577     226.59
 C      -0.575421     2.185376     2.346192      91.85
 H      -0.135672     3.115732     1.517632      20.09
 H      -1.435306     2.372614     2.945983      23.45
 H       0.328823     2.199729     3.031675      22.92
 C      -0.732059    -0.578320    -0.099473      -2.68
 O      -2.125332    -0.500380    -0.022249     127.03
 C      -0.005874    -1.167705    -1.163914      62.38
 H      -0.624598    -1.589774    -1.838639      22.03
 C       2.194017    -0.232226    -0.298796      14.99
 C       3.589512     0.180720    -0.547293      75.67
 H       3.778437    -0.107188    -1.638502      18.87
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 O       3.829012     1.573985    -0.320924     265.73
 H       3.900259     1.736741     0.691271      20.04
 C       4.612826    -0.853843     0.300848      77.75
 H       4.633599    -0.544221     1.420536      17.96
 O       4.259968    -2.250072     0.177178     289.50
 H       3.870667    -2.330628    -0.734943      24.81
 C       6.119711    -0.856515    -0.041232      59.15
 O       6.839295     0.534494     0.286963     302.67
 H       6.663877     0.615418     1.296506      27.93
 H       6.048145    -1.163403    -1.123652      27.39
 H       6.451474    -1.611108     0.864865      26.00
55
name= lig-ACN-Water-frame_779
 C      -3.835971     1.441526    -3.022696      62.21
 H      -3.624691     0.717363    -3.700866      22.90
 C      -3.813965     2.223875    -0.799545      22.91
 H      -3.721088     2.080193     0.417688      15.58
 C      -3.663092     3.678817    -1.221503      12.24
 O      -3.173209     4.640164    -0.212910     254.33
 C      -3.291529     4.417934     1.170681      55.39
 H      -2.892382     5.242460     1.798152      19.95
 H      -2.674576     3.555797     1.502170      25.74
 H      -4.290949     4.337680     1.595695      23.63
 C      -3.657000     3.885562    -2.589490     -11.08
 O      -3.211325     5.153725    -3.206765     103.99
 H      -3.265306     5.871850    -2.529557      26.33
 C      -3.592135     2.723544    -3.498052      57.29
 H      -3.508081     3.024899    -4.622308      21.01
 C      -4.083418     1.092437    -1.703135      30.83
 C      -4.244698    -0.307385    -1.121361      93.89
 H      -4.920933    -0.848127    -1.705048      22.68
 O      -4.894278    -0.438512     0.239251     216.55
 H      -4.266679    -0.077343     1.015814      20.71
 C      -2.904511    -1.128960    -1.114131      70.47
 H      -2.194725    -0.974440    -1.993592      22.22
 C      -3.147483    -2.705699    -0.846832     111.65
 O      -4.278799    -3.109949    -1.402042     257.08
 H      -4.163890    -3.483994    -2.409312      25.47
 H      -3.227261    -2.740435     0.240295      24.82
 H      -2.423196    -3.428364    -1.176443      22.94
 C       1.386595    -1.036052    -1.245609      42.86
 H       1.845244    -1.617944    -2.047109      19.65
 C       1.485796     0.380320     0.812341      95.45
 H       1.865841     1.136175     1.528411       9.56
 C       0.074319     0.209064     0.796957      13.66
 O      -0.813848     0.796814     1.689285     151.48
 C      -0.436419     2.241618     2.314982      70.95
 H      -0.292661     3.220325     1.428772      18.44
 H      -1.517359     2.442551     2.551925      18.78
 H       0.206591     2.225687     3.257616      20.88
 C      -0.675495    -0.479065    -0.210720       5.35
 O      -2.109071    -0.605962     0.019301     148.56
 C      -0.014208    -1.110085    -1.278131      71.67
 H      -0.329893    -1.835464    -2.020516      19.54
 C       2.082672    -0.292750    -0.246443      48.40
 C       3.608835     0.154755    -0.497134      79.98
 H       3.819515     0.056621    -1.588468      21.59
 O       3.858050     1.599519    -0.356287     249.75
 H       4.017357     1.819396     0.634470      20.46
 C       4.583566    -0.742768     0.291761     110.31
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 H       4.351002    -0.487328     1.368152      24.15
 O       4.318669    -2.199468     0.279490     266.10
 H       3.997113    -2.492102    -0.655313      26.35
 C       6.139412    -0.737941     0.007603      94.35
 O       6.721217     0.504029     0.244581     294.90
 H       6.878142     0.793387     1.166638      30.83
 H       6.736379    -0.912178    -0.908478      26.57
 H       6.624625    -1.716039     0.574694      26.47
55
name= lig-ACN-Water-frame_780
 C      -3.747434     1.378585    -3.120758      50.19
 H      -3.849133     0.703982    -3.857898      22.70
 C      -3.863921     2.268351    -0.755619      68.24
 H      -3.748098     1.913160     0.352845      16.57
 C      -3.660518     3.571096    -1.071172      21.07
 O      -3.145479     4.592929    -0.345002     227.30
 C      -3.294897     4.386077     1.160582      31.90
 H      -2.843365     5.409089     1.330382      20.04
 H      -2.696027     3.620006     1.466921      27.45
 H      -4.401704     4.134374     1.380048      25.50
 C      -3.548690     3.884205    -2.530013      24.67
 O      -3.254207     5.000494    -3.216130     177.09
 H      -3.108801     5.785722    -2.532472      24.17
 C      -3.734353     2.807105    -3.364406      51.46
 H      -3.635656     2.997232    -4.414889      25.40
 C      -3.932973     1.174866    -1.638664       8.73
 C      -4.231264    -0.332294    -1.066919      91.16
 H      -4.788866    -0.848156    -1.737635      24.90
 O      -4.912838    -0.436190     0.159866     244.77
 H      -4.296074    -0.179556     0.943377      23.45
 C      -2.796837    -1.175175    -1.033326      70.10
 H      -2.418172    -1.003722    -2.160955      20.78
 C      -3.086167    -2.681418    -0.750271     103.89
 O      -4.414888    -3.173320    -1.391292     277.43
 H      -4.131396    -3.797373    -2.006421      29.76
 H      -3.210670    -2.887910     0.348215      25.34
 H      -2.169967    -3.145916    -1.020750      24.65
 C       1.443029    -1.079904    -1.161443      37.18
 H       2.164043    -1.527716    -1.854592      20.43
 C       1.415003     0.401125     0.794081      20.90
 H       2.016101     0.866135     1.643663      12.81
 C       0.003032     0.441349     0.666392      12.39
 O      -0.861532     0.864218     1.685307     237.90
 C      -0.459581     2.170972     2.220463      71.29
 H       0.317190     2.484055     1.331998      19.29
 H      -1.419719     2.786957     2.703457      19.57
 H       0.402933     1.958199     3.024340      23.73
 C      -0.712647    -0.461869    -0.285707       1.68
 O      -1.979224    -0.686262     0.016350     180.52
 C       0.027577    -1.116382    -1.312779      65.28
 H      -0.596290    -1.689875    -2.130245      18.12
 C       2.181485    -0.238468    -0.282090      35.35
 C       3.617247     0.035429    -0.571233      79.98
 H       3.798661    -0.075516    -1.632364      22.08
 O       3.877002     1.571159    -0.336377     174.96
 H       4.185856     1.662857     0.605886      21.84
 C       4.668658    -0.725922     0.332633     101.58
 H       4.576014    -0.399373     1.362019      22.87
 O       4.271730    -2.164197     0.340521     271.46
 H       4.490860    -2.501299    -0.550896      30.29
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 C       6.156113    -0.678606     0.016217      92.43
 O       6.700758     0.623204     0.237570     277.87
 H       6.585127     0.793817     1.195158      31.56
 H       5.945800    -1.061595    -0.969136      29.44
 H       6.640724    -1.366704     0.862878      28.28
55
name= lig-ACN-Water-frame_781
 C      -3.795296     1.430883    -2.955606      61.55
 H      -4.015389     0.646363    -3.613096      23.80
 C      -3.903996     2.173497    -0.647161      59.67
 H      -4.122646     2.044108     0.407005      17.64
 C      -3.522988     3.513408    -1.147717      14.26
 O      -3.166651     4.569246    -0.352774     233.05
 C      -3.256032     4.425925     1.045546      65.15
 H      -3.059184     5.305089     1.826517      19.77
 H      -2.747161     3.676064     1.441916      29.95
 H      -4.413303     4.301026     1.313921      23.43
 C      -3.495083     3.702385    -2.480255      24.78
 O      -3.269146     4.972859    -3.160883     182.49
 H      -3.445086     5.785577    -2.619101      25.06
 C      -3.811476     2.747834    -3.442780      70.17
 H      -3.834720     3.124136    -4.362227      28.06
 C      -3.816587     1.125376    -1.611245      24.08
 C      -4.067024    -0.317506    -1.116432      96.39
 H      -4.632713    -0.735187    -1.847328      27.13
 O      -4.951614    -0.417677     0.088537     184.56
 H      -4.472812    -0.125287     0.879002      24.96
 C      -2.940003    -1.215724    -1.009094      86.63
 H      -2.350544    -1.167507    -2.089280      22.24
 C      -3.082287    -2.687994    -0.682551      96.85
 O      -4.429910    -3.238338    -1.353563     238.76
 H      -4.166110    -3.947221    -1.964495      28.32
 H      -3.280866    -2.671534     0.469052      24.11
 H      -2.293469    -3.322986    -1.031814      24.32
 C       1.551348    -1.058639    -1.235593      57.63
 H       1.944820    -1.613523    -2.107130      18.99
 C       1.322837     0.431041     0.661671      50.97
 H       1.769799     0.949694     1.580564      15.94
 C      -0.092223     0.444851     0.618309      15.78
 O      -0.915930     0.936585     1.644620     225.56
 C      -0.330800     2.088404     2.180586     122.87
 H       0.056001     2.890499     1.413749      22.77
 H      -1.231384     2.887799     2.550021      19.62
 H       0.291999     1.845866     3.164911      24.87
 C      -0.574736    -0.385474    -0.314338      20.11
 O      -1.933679    -0.736963     0.001735     139.54
 C       0.156693    -1.120848    -1.234223      55.61
 H      -0.385308    -1.785968    -2.112297      19.51
 C       2.163845    -0.199311    -0.269433      34.99
 C       3.719029     0.086543    -0.547563      81.79
 H       3.897331    -0.325521    -1.485853      25.99
 O       3.902487     1.449497    -0.363648     252.97
 H       3.877027     1.606482     0.612202      22.97
 C       4.600447    -0.779687     0.455986      91.07
 H       4.441426    -0.459363     1.432130      25.08
 O       4.248999    -2.137288     0.386840     292.66
 H       4.656896    -2.557030    -0.392334      31.89
 C       6.104852    -0.682933     0.011514      97.34
 O       6.705621     0.781548     0.209954     184.40
 H       6.688370     0.955067     1.223774      29.25
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 H       6.575787    -0.800043    -0.956050      29.20
 H       6.730031    -1.505834     0.579497      28.87
55
name= lig-ACN-Water-frame_782
 C      -3.927586     1.371636    -2.873092      44.58
 H      -3.889983     0.508738    -3.602626      22.23
 C      -3.825248     2.180935    -0.560904      73.16
 H      -4.157139     2.050220     0.370467      17.83
 C      -3.404504     3.377128    -1.096683      -0.55
 O      -3.158414     4.631234    -0.363314     216.55
 C      -3.331613     4.427695     1.083416      17.73
 H      -2.759592     5.479313     1.266286      20.84
 H      -2.743020     3.648693     1.309952      30.33
 H      -4.453733     4.147434     1.436971      23.28
 C      -3.470651     3.722845    -2.651337       3.30
 O      -3.277939     4.980089    -3.044480     152.43
 H      -3.760280     5.512840    -2.441684      27.74
 C      -3.802978     2.626208    -3.535010      59.74
 H      -4.075914     2.575444    -4.468292      24.84
 C      -3.799766     1.088703    -1.467162      33.30
 C      -4.129115    -0.323442    -1.158071      94.36
 H      -4.689941    -0.739730    -1.914529      25.64
 O      -4.982981    -0.386556    -0.002943     219.90
 H      -4.528803     0.035351     0.740249      25.04
 C      -2.815213    -1.279114    -1.057195      66.10
 H      -2.260435    -1.266956    -2.180182      20.87
 C      -3.292605    -2.778701    -0.658601      99.81
 O      -4.333106    -3.280337    -1.254289     290.50
 H      -4.006608    -3.805491    -2.166987      24.67
 H      -3.374369    -2.929170     0.542311      22.71
 H      -2.318267    -3.334871    -0.831872      22.29
 C       1.629366    -0.968631    -1.375091      40.85
 H       2.421645    -1.446954    -2.019828      18.28
 C       1.348114     0.553048     0.605207      81.97
 H       1.855836     1.290885     1.273394      18.51
 C      -0.038459     0.362119     0.670218       0.57
 O      -0.942974     0.966631     1.506952     150.03
 C      -0.270051     2.238399     2.287572      66.95
 H       0.242642     2.638988     1.481149      23.93
 H      -1.351388     2.502068     2.835098      19.96
 H       0.677270     1.902298     3.000354      22.20
 C      -0.690242    -0.490375    -0.363087      11.89
 O      -1.959920    -0.780058    -0.044747     193.92
 C       0.226630    -1.166248    -1.205783      55.96
 H      -0.261282    -2.080050    -1.891694      20.09
 C       2.193751    -0.221255    -0.377499      32.03
 C       3.651220     0.018311    -0.385182     102.11
 H       4.011799    -0.104431    -1.341531      24.37
 O       3.972114     1.443887    -0.412175     232.18
 H       3.975456     1.861642     0.493300      25.58
 C       4.612639    -0.772600     0.473939     100.46
 H       4.527171    -0.545096     1.458562      27.48
 O       4.207814    -2.210023     0.446242     272.48
 H       4.499613    -2.632941    -0.443118      29.43
 C       6.217561    -0.507752     0.053398      96.73
 O       6.624716     0.767916     0.247767     264.03
 H       6.920253     0.903326     1.246112      26.37
 H       6.079841    -0.825198    -0.992348      30.76
 H       6.801570    -1.207193     0.727596      28.16
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name= lig-ACN-Water-frame_783
 C      -3.947453     1.256680    -2.866649      45.81
 H      -4.212816     0.255209    -3.462562      21.31
 C      -3.665935     2.198040    -0.543332      56.05
 H      -3.638554     2.135304     0.447833      16.69
 C      -3.346029     3.484480    -1.220019      14.77
 O      -3.221038     4.559826    -0.457270     176.94
 C      -3.298383     4.464588     1.088502      51.25
 H      -2.989340     5.432559     1.730493      21.59
 H      -2.753256     3.689147     1.565698      29.30
 H      -4.506758     4.487330     1.389817      24.58
 C      -3.458735     3.595658    -2.599321     -12.65
 O      -3.311017     5.045770    -2.967680     135.30
 H      -3.545848     5.670924    -2.211616      22.68
 C      -3.783350     2.515745    -3.472776      62.46
 H      -3.820253     2.772108    -4.470468      19.54
 C      -3.910318     1.106953    -1.489437      14.60
 C      -4.170540    -0.440590    -1.166883      78.86
 H      -4.768948    -0.858506    -1.958750      25.18
 O      -5.035666    -0.397128    -0.032709     206.40
 H      -4.520747    -0.181267     0.840423      22.69
 C      -2.884761    -1.389977    -1.090770      75.81
 H      -2.327051    -1.421691    -2.210872      20.27
 C      -3.159194    -2.774740    -0.526870      86.72
 O      -4.399505    -3.420008    -1.296498     254.76
 H      -4.120468    -3.489839    -2.259114      28.37
 H      -3.737799    -2.489473     0.557108      21.05
 H      -2.341754    -3.545162    -0.519816      22.32
 C       1.613453    -0.906679    -1.396609      70.20
 H       2.084298    -1.492532    -2.253901      18.65
 C       1.412250     0.599853     0.510435      54.87
 H       1.933220     1.306318     1.130461      16.49
 C       0.023842     0.294257     0.618611      -0.41
 O      -0.856831     1.086103     1.463325     197.45
 C      -0.327158     2.202110     2.289011      95.82
 H      -0.225089     3.101119     1.824147      24.13
 H      -0.937170     2.835358     3.160720      22.67
 H       0.680971     1.735528     2.911173      21.84
 C      -0.566424    -0.645323    -0.273074      -0.28
 O      -2.009116    -0.823268    -0.089518     154.85
 C       0.168672    -1.304717    -1.320100      47.75
 H      -0.364944    -2.174636    -1.983326      17.66
 C       2.178572    -0.085000    -0.360693      38.39
 C       3.712007     0.028908    -0.424020      78.09
 H       3.800022    -0.488605    -1.299990      26.52
 O       4.044639     1.545642    -0.425093     161.57
 H       4.272136     1.657310     0.543887      23.47
 C       4.699489    -0.825120     0.606838      94.89
 H       4.559955    -0.573039     1.588827      26.63
 O       4.221890    -2.260152     0.493327     267.33
 H       4.175552    -2.422549    -0.474640      28.26
 C       6.103651    -0.572198     0.114922     104.55
 O       6.605203     0.875157     0.301807     264.35
 H       6.739512     0.975074     1.349052      26.70
 H       6.395489    -0.700140    -0.981650      28.51
 H       6.849678    -1.245536     0.601793      28.72
55
name= lig-ACN-Water-frame_784
 C      -3.963237     1.226492    -2.914748      26.44
 H      -4.414721     0.455030    -3.787119      18.09
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 C      -3.473805     2.099673    -0.734058      68.60
 H      -3.214431     1.949458     0.289435      21.79
 C      -3.430532     3.388171    -1.148200      11.54
 O      -3.222447     4.596043    -0.398926     243.42
 C      -3.318137     4.539887     1.006663      42.83
 H      -2.800592     5.542043     1.198896      20.65
 H      -2.693281     3.640249     1.390251      25.53
 H      -4.536196     4.269597     1.266042      20.77
 C      -3.454798     3.688942    -2.548958      31.34
 O      -3.357378     4.963395    -2.994033     143.05
 H      -3.387296     5.535361    -2.091843      18.49
 C      -3.702944     2.570415    -3.388964      50.88
 H      -3.657877     2.672532    -4.505186      24.31
 C      -3.957685     0.994588    -1.507610      35.31
 C      -4.189165    -0.448700    -1.127287      91.16
 H      -4.838672    -0.880401    -1.935417      23.98
 O      -5.106475    -0.505625     0.046800     201.44
 H      -4.554902    -0.337650     0.899052      24.11
 C      -2.980810    -1.454064    -1.085261      59.40
 H      -2.498039    -1.495449    -2.218001      21.19
 C      -3.265999    -2.809019    -0.481182      84.10
 O      -4.375290    -3.531666    -1.299978     270.54
 H      -4.168597    -3.527267    -2.184485      31.25
 H      -3.718812    -2.685008     0.709179      21.74
 H      -2.289544    -3.484420    -0.331004      22.54
 C       1.481274    -0.947869    -1.359691      39.94
 H       2.168661    -1.187267    -2.201611      21.59
 C       1.391532     0.637410     0.529628      70.81
 H       1.666619     1.405899     1.198479      12.63
 C       0.028157     0.383552     0.589963      -1.45
 O      -0.800769     1.154799     1.407617     209.05
 C      -0.338036     2.174600     2.297515      90.08
 H      -0.191777     3.000062     1.770266      25.11
 H      -1.173502     1.730150     2.982902      18.84
 H       0.868669     2.017757     2.719333      21.46
 C      -0.562415    -0.803107    -0.205977       2.53
 O      -1.926430    -0.811841    -0.091425      99.80
 C       0.160620    -1.313866    -1.291371      75.91
 H      -0.212821    -1.855196    -2.219647      20.84
 C       2.222792    -0.096833    -0.512704      26.46
 C       3.815718     0.120626    -0.488461      81.64
 H       4.398465    -0.016370    -1.343866      18.40
 O       4.109562     1.517812    -0.455636     202.82
 H       4.413297     1.873561     0.404108      21.36
 C       4.579941    -0.827299     0.619947      90.69
 H       4.537890    -0.610786     1.646523      23.84
 O       4.312221    -2.230800     0.524327     312.88
 H       3.843124    -2.367602    -0.306137      28.84
 C       6.138661    -0.655471     0.195404      76.08
 O       6.570289     0.923758     0.345214     263.13
 H       6.684299     1.158252     1.334424      28.33
 H       6.149086    -0.701895    -0.974278      27.50
 H       6.749380    -1.290071     0.750399      29.15
55
name= lig-ACN-Water-frame_785
 C      -4.022953     1.370594    -2.971241      56.07
 H      -4.246466     0.510742    -3.852510      24.96
 C      -3.367893     1.885160    -0.747957      28.70
 H      -3.171175     1.496926     0.327799      20.54
 C      -3.466825     3.402616    -1.120859       4.75
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 O      -3.211670     4.563289    -0.453418     210.29
 C      -3.313471     4.586723     0.973115      68.19
 H      -3.034631     5.536586     1.435809      20.62
 H      -2.516122     3.851624     1.511691      24.47
 H      -4.443729     4.530245     1.577783      21.59
 C      -3.511338     3.644388    -2.497772      20.08
 O      -3.385429     4.923167    -3.069251     172.39
 H      -3.345686     5.726992    -2.458085      24.60
 C      -3.618617     2.603586    -3.395732      66.70
 H      -3.706819     2.863102    -4.564682      18.29
 C      -3.848322     0.892694    -1.656644      21.49
 C      -4.282830    -0.487839    -1.030297      92.94
 H      -4.916794    -1.003142    -1.861934      23.74
 O      -5.116744    -0.638012     0.141690     175.32
 H      -4.706381    -0.198856     0.900353      26.93
 C      -2.969543    -1.398393    -0.950039      65.50
 H      -2.558446    -1.574216    -2.073189      22.24
 C      -3.459942    -2.914754    -0.494193      86.20
 O      -4.302309    -3.602556    -1.235199     262.93
 H      -3.800922    -3.918138    -2.117636      24.71
 H      -3.896106    -2.968440     0.687657      21.96
 H      -2.380253    -3.410662    -0.615978      20.99
 C       1.654073    -0.970815    -1.408538      57.11
 H       2.021808    -1.460940    -2.304465      18.79
 C       1.447501     0.573261     0.436391      68.73
 H       2.058265     1.309374     0.917110      16.86
 C       0.059294     0.328818     0.515021      12.07
 O      -0.820515     1.084926     1.260376     172.71
 C      -0.347573     2.114734     2.344352      95.18
 H      -0.634104     2.954030     2.047334      26.04
 H      -0.890584     2.306160     3.357225      23.66
 H       0.870618     1.969839     2.715790      20.24
 C      -0.607800    -0.697487    -0.193302       9.99
 O      -1.997774    -0.836617    -0.076258     167.55
 C       0.142427    -1.283990    -1.210890      38.77
 H      -0.468330    -1.808174    -1.921598      20.93
 C       2.251609    -0.037003    -0.482210      23.70
 C       3.800334     0.135659    -0.552333      85.61
 H       3.921068    -0.385937    -1.523190      23.58
 O       4.153293     1.564106    -0.479034     257.57
 H       4.254927     1.683337     0.491260      25.21
 C       4.610878    -0.704944     0.537372      83.75
 H       4.112965    -0.301401     1.403929      24.24
 O       4.353093    -2.200776     0.531160     289.00
 H       3.700189    -2.408814    -0.217470      27.74
 C       6.126547    -0.513093     0.308018     113.47
 O       6.536372     0.794060     0.358114     407.64
 H       6.657789     0.866618     1.308678      34.14
 H       6.301930    -1.076679    -0.659540      29.62
 H       6.748413    -1.094978     0.934934      28.37
55
name= lig-ACN-Water-frame_786
 C      -4.029085     1.299950    -3.071217      40.42
 H      -4.363558     0.490793    -3.926270      24.75
 C      -3.394045     1.924006    -0.715086      71.14
 H      -3.133419     1.757898     0.461111      16.92
 C      -3.396224     3.208476    -1.111533      20.41
 O      -3.223443     4.514650    -0.450894     184.12
 C      -3.275738     4.673747     1.085475      42.87
 H      -3.036796     5.656123     1.149215      21.88
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 H      -2.489743     3.825744     1.603812      22.39
 H      -4.426466     4.166742     1.103134      21.52
 C      -3.535109     3.621242    -2.506630      -2.51
 O      -3.407164     4.930710    -3.161429     158.73
 H      -3.494598     5.562077    -2.480384      28.12
 C      -3.655703     2.643471    -3.498528      29.76
 H      -3.594946     3.107539    -4.653983      18.39
 C      -3.805488     0.922891    -1.657020      18.07
 C      -4.259812    -0.574597    -1.081132      73.95
 H      -4.955313    -1.188404    -1.836060      22.52
 O      -5.088977    -0.668617     0.215248     125.29
 H      -4.591635    -0.144234     0.886310      25.46
 C      -3.083463    -1.466563    -0.862068      83.01
 H      -2.577149    -1.445144    -1.916967      22.76
 C      -3.311014    -2.910671    -0.398709      81.45
 O      -4.354240    -3.724740    -1.320788     178.77
 H      -3.768351    -4.314060    -2.039058      23.60
 H      -3.890407    -2.751761     0.653945      23.19
 H      -2.389975    -3.639602    -0.063249      22.67
 C       1.593865    -1.031271    -1.413888      54.35
 H       2.244357    -1.531224    -2.091122      21.92
 C       1.493707     0.558726     0.382181      66.73
 H       1.704798     1.328945     1.145630      17.65
 C       0.071757     0.336176     0.561673      -8.70
 O      -0.867029     1.100194     1.313597     200.45
 C      -0.389569     2.057196     2.303822     115.58
 H      -0.432220     2.932039     1.975446      27.46
 H      -0.904559     1.548245     3.168012      23.71
 H       0.823489     1.938026     2.283471      22.77
 C      -0.606485    -0.573595    -0.337602     -29.71
 O      -2.089939    -0.832921     0.057130      96.90
 C       0.276028    -1.268801    -1.214835      71.06
 H      -0.019080    -2.088763    -1.731310      25.53
 C       2.286462    -0.176208    -0.568890      33.55
 C       3.740608     0.086714    -0.678738      84.95
 H       4.238276     0.036861    -1.723335      18.92
 O       4.144989     1.567728    -0.521813     194.14
 H       4.342490     1.828878     0.419561      22.94
 C       4.546640    -0.623680     0.446290      98.93
 H       4.419064    -0.278175     1.501572      22.57
 O       4.375188    -2.096938     0.515338     283.71
 H       3.692588    -2.335922    -0.131204      28.99
 C       6.091007    -0.591843     0.430666     102.72
 O       6.606233     0.778537     0.381843     341.08
 H       6.609340     1.263739     1.199468      32.04
 H       6.546357    -0.979512    -0.521704      27.46
 H       6.267639    -1.126549     1.279415      30.29
55
name= lig-ACN-Water-frame_787
 C      -3.929291     1.205853    -3.041581      45.72
 H      -4.383459     0.422930    -3.772871      19.66
 C      -3.500594     1.967373    -0.711544      38.86
 H      -3.310466     1.666906     0.431624      18.31
 C      -3.307855     3.373647    -1.212283       4.35
 O      -3.190737     4.408542    -0.391740     235.98
 C      -3.312873     4.624374     0.995273      86.34
 H      -3.189572     5.611430     1.176677      20.46
 H      -2.327755     4.157484     1.638005      20.75
 H      -4.303722     4.555819     1.774229      21.65
 C      -3.487073     3.614077    -2.671167      28.70
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 O      -3.438158     4.874154    -3.127186     171.91
 H      -3.545782     5.623464    -2.465419      23.28
 C      -3.795645     2.546955    -3.532451      53.61
 H      -3.805813     2.644601    -4.772073      24.15
 C      -3.914726     0.882975    -1.657698      13.79
 C      -4.257478    -0.588105    -1.077694      77.19
 H      -4.998409    -0.986333    -1.945400      23.61
 O      -5.019348    -0.578262     0.179043     166.97
 H      -4.363471    -0.333249     0.955205      23.25
 C      -2.968848    -1.588616    -0.944025      52.35
 H      -2.443656    -1.734805    -1.933774      21.99
 C      -3.338599    -2.997656    -0.338905      80.85
 O      -4.283095    -3.756602    -1.300922     251.54
 H      -3.744973    -3.999511    -2.082779      27.41
 H      -4.019814    -2.929111     0.578583      23.17
 H      -2.176934    -3.414111    -0.151213      21.74
 C       1.626430    -1.118513    -1.418989      48.35
 H       2.084923    -1.729340    -2.193103      20.02
 C       1.409260     0.562920     0.422623      97.94
 H       2.215210     1.177488     0.882626      14.64
 C      -0.005481     0.401666     0.484159       9.83
 O      -0.857032     1.052734     1.323718     189.26
 C      -0.329465     1.963018     2.281768     111.90
 H      -0.781497     2.805154     2.054024      24.72
 H      -0.875858     1.842781     3.271897      23.40
 H       0.741550     1.853890     2.604977      23.48
 C      -0.692414    -0.566744    -0.376827     -17.51
 O      -1.975024    -0.817969     0.140517      89.06
 C       0.145974    -1.400233    -1.279348      45.35
 H      -0.308921    -2.128580    -1.814605      23.01
 C       2.245265    -0.129408    -0.552296      20.98
 C       3.839150     0.187136    -0.715244      85.92
 H       4.219816    -0.358485    -1.735205      23.31
 O       4.053644     1.558105    -0.608715     198.41
 H       4.264937     1.671418     0.363264      28.56
 C       4.556853    -0.637550     0.396461      95.24
 H       3.895647    -0.110266     1.193566      25.74
 O       4.324572    -2.012635     0.484519     298.48
 H       3.641119    -2.307216    -0.120266      29.59
 C       6.102449    -0.620949     0.504500      99.54
 O       6.745556     0.828815     0.425254     296.31
 H       6.658746     1.003759     1.436499      27.82
 H       6.473004    -1.290269    -0.297883      28.25
 H       6.409068    -1.038636     1.403248      28.89
55
name= lig-ACN-Water-frame_788
 C      -3.921985     1.088491    -2.945896      47.19
 H      -4.001568     0.262952    -3.651673      21.31
 C      -3.650136     2.030737    -0.866258      74.72
 H      -3.702113     2.012722     0.255278      17.65
 C      -3.359330     3.263800    -1.306274      17.48
 O      -3.154871     4.429084    -0.456686     221.07
 C      -3.305656     4.621281     1.015906      39.98
 H      -3.102228     5.651380     1.093379      20.70
 H      -2.453063     3.876269     1.536249      22.68
 H      -4.413465     4.078784     1.141627      21.65
 C      -3.452627     3.519708    -2.681276       7.17
 O      -3.450738     4.898667    -3.162821      56.80
 H      -3.706817     5.438994    -2.276173      21.53
 C      -3.873529     2.385057    -3.518253      -4.57
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 H      -4.209768     2.576986    -4.658716      21.17
 C      -3.926935     0.899992    -1.560876      47.31
 C      -4.166128    -0.538079    -1.096744      90.37
 H      -4.902427    -1.210284    -1.771998      22.64
 O      -4.927700    -0.471534     0.094560     216.56
 H      -4.347688    -0.127131     0.911867      20.58
 C      -2.908687    -1.584212    -0.919462      77.07
 H      -2.362715    -1.737717    -1.811431      23.88
 C      -3.386520    -3.033112    -0.384006      98.68
 O      -4.114145    -3.744172    -1.234833     327.76
 H      -3.838187    -3.614683    -2.087009      31.82
 H      -3.829437    -2.970540     0.600951      24.16
 H      -2.450225    -3.869056    -0.155045      21.39
 C       1.440789    -1.196502    -1.380196      48.43
 H       2.110786    -1.554101    -2.192052      23.12
 C       1.425715     0.555048     0.355543      75.54
 H       1.510397     1.353450     1.097916      13.31
 C       0.001583     0.417650     0.332263       7.52
 O      -0.836549     0.953179     1.324918     189.33
 C      -0.324332     1.972194     2.394347     126.35
 H      -0.331021     2.846575     2.056965      27.67
 H      -0.840786     1.652542     3.297017      23.95
 H       0.712328     2.005261     2.386095      25.54
 C      -0.594937    -0.669023    -0.329009      17.60
 O      -1.928851    -0.927557     0.011534     145.76
 C       0.047819    -1.403873    -1.270939      72.29
 H      -0.440808    -2.043631    -1.949469      22.07
 C       2.166345    -0.139110    -0.603776      16.01
 C       3.762531     0.103370    -0.741547      70.82
 H       3.854004    -0.063292    -1.932705      21.23
 O       3.994025     1.598106    -0.704629     199.13
 H       4.154207     1.912046     0.208249      26.28
 C       4.567932    -0.541806     0.459535      84.75
 H       4.335681    -0.205061     1.572806      23.45
 O       4.220842    -2.039740     0.435062     276.52
 H       3.471880    -2.126063    -0.252192      26.04
 C       6.174498    -0.469700     0.565704     105.16
 O       6.836511     0.745319     0.501173     297.12
 H       7.174515     1.166269     1.383156      28.39
 H       6.622529    -1.034561    -0.290840      28.48
 H       6.376379    -1.019274     1.474716      29.11
55
name= lig-ACN-Water-frame_789
 C      -3.959889     0.989498    -3.011179      58.91
 H      -3.951740     0.162279    -3.588253      22.99
 C      -3.804176     2.035623    -0.691538      53.39
 H      -3.971322     1.964144     0.334665      15.59
 C      -3.427263     3.310494    -1.307676       9.76
 O      -3.085020     4.455931    -0.676811     177.91
 C      -3.319315     4.463779     0.899181      68.32
 H      -3.285541     5.521834     1.257913      22.26
 H      -2.600723     3.852927     1.615218      25.80
 H      -4.431256     4.309005     1.230122      25.33
 C      -3.534914     3.491809    -2.767256      18.00
 O      -3.464805     4.805623    -3.199385     114.54
 H      -3.713772     5.456862    -2.456212      26.65
 C      -3.860919     2.362125    -3.481660      68.84
 H      -4.096527     2.528364    -4.576491      22.37
 C      -3.844049     0.816591    -1.612698      13.19
 C      -4.039920    -0.572573    -1.044087      97.52
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 H      -4.670534    -0.997234    -1.941687      23.00
 O      -4.906959    -0.400419     0.099888     224.90
 H      -4.397008     0.063540     0.812713      23.33
 C      -2.898928    -1.554615    -0.907470      98.52
 H      -2.624830    -1.646093    -1.897417      23.35
 C      -3.209400    -2.958124    -0.298123      80.16
 O      -4.133455    -3.764626    -1.285365     215.55
 H      -3.633478    -3.851531    -2.228026      24.26
 H      -3.861652    -2.790800     0.472588      24.30
 H      -2.068603    -3.299778     0.083644      21.77
 C       1.435271    -1.124924    -1.393448      46.44
 H       1.858868    -1.777065    -2.213439      22.07
 C       1.346245     0.627419     0.242660      65.25
 H       2.071718     1.237991     0.731964      16.90
 C       0.002905     0.360160     0.415591      10.10
 O      -0.791507     0.942820     1.392475     205.88
 C      -0.281648     1.921794     2.340177     136.34
 H      -0.544467     2.785975     2.149428      26.57
 H      -0.963302     1.754956     3.171151      23.17
 H       0.578375     1.579946     2.666798      25.96
 C      -0.661338    -0.768275    -0.299842       5.97
 O      -1.942609    -1.035601    -0.060030     173.24
 C       0.096964    -1.422745    -1.321307      59.65
 H      -0.337505    -2.279978    -1.957588      18.64
 C       2.114688    -0.233380    -0.626744      44.56
 C       3.583924     0.144648    -0.711330      96.69
 H       4.328962    -0.394111    -1.384105      21.05
 O       3.952494     1.604573    -0.793454     221.32
 H       3.968106     1.885835     0.152443      25.44
 C       4.562224    -0.571696     0.480305      63.43
 H       3.989830    -0.090956     1.435635      20.67
 O       4.167208    -1.996750     0.404274     281.55
 H       3.506359    -2.021625    -0.311416      27.18
 C       6.185306    -0.504202     0.559607      90.09
 O       6.969901     0.795196     0.568488     320.76
 H       6.816269     1.056103     1.516667      28.54
 H       6.573168    -1.046631    -0.374605      26.63
 H       6.394866    -1.061848     1.453085      26.48
55
name= lig-ACN-Water-frame_790
 C      -3.907607     1.036695    -3.032676      54.95
 H      -4.158731     0.368658    -3.687260      23.80
 C      -3.842011     1.989335    -0.700404      70.00
 H      -3.876017     1.866652     0.276072       9.97
 C      -3.546761     3.269509    -1.293886      30.85
 O      -3.054854     4.473355    -0.695982     271.05
 C      -3.348194     4.386490     0.675544      48.17
 H      -2.906896     5.445654     1.044832      19.42
 H      -2.604630     3.608912     0.922567      30.85
 H      -4.296244     3.971620     0.852583      29.85
 C      -3.656211     3.411107    -2.671715       4.95
 O      -3.478016     4.694681    -3.306574     171.73
 H      -3.635787     5.283655    -2.595362      29.95
 C      -3.850771     2.331507    -3.626707      41.27
 H      -3.800568     2.444468    -4.671127      23.12
 C      -3.771774     0.889021    -1.586163      39.41
 C      -4.114104    -0.566002    -1.029764     102.59
 H      -4.885293    -1.197381    -1.626426      23.52
 O      -4.929631    -0.401199     0.155689     208.83
 H      -4.378370    -0.294193     0.923732      24.30
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 C      -2.903868    -1.594478    -1.027772      87.72
 H      -2.415471    -1.715870    -1.874555      23.28
 C      -3.226577    -2.888419    -0.352381     100.16
 O      -4.051319    -3.729303    -1.233531     260.46
 H      -3.442475    -4.183218    -2.034829      24.75
 H      -3.649695    -2.833869     0.545331      25.64
 H      -2.238141    -3.627170    -0.163368      20.14
 C       1.549155    -1.179222    -1.567661      49.99
 H       2.317659    -1.695936    -2.224902      18.47
 C       1.327962     0.637174     0.162943      58.25
 H       1.597827     1.535332     0.680297      19.47
 C      -0.020964     0.227644     0.545265      -0.21
 O      -0.813384     0.915833     1.413430     212.84
 C      -0.302165     1.837999     2.361540     139.36
 H      -0.095525     2.628151     1.899947      28.46
 H      -0.953055     1.903659     3.211317      24.15
 H       0.648124     1.792346     2.628970      28.17
 C      -0.621554    -0.746124    -0.336852       8.34
 O      -1.942435    -1.028262     0.071319     166.92
 C       0.102818    -1.452406    -1.293337      50.62
 H      -0.482798    -2.310276    -1.918905      19.00
 C       2.136166    -0.158051    -0.649044       8.59
 C       3.717458     0.113210    -0.673224      89.18
 H       3.695434    -0.164293    -1.753336      20.29
 O       3.903166     1.509264    -0.814469     240.43
 H       4.076013     1.970527     0.050654      25.39
 C       4.423219    -0.548920     0.493910      78.62
 H       4.131916    -0.266244     1.658195      20.93
 O       4.167754    -1.934973     0.408888     274.65
 H       3.723277    -2.205585    -0.403450      27.94
 C       6.122663    -0.555636     0.473264      73.32
 O       7.000160     0.799724     0.667078     237.05
 H       6.850592     1.195795     1.526489      28.04
 H       6.469666    -1.025719    -0.507497      26.38
 H       6.533120    -1.167303     1.335524      25.64
55
name= lig-ACN-Water-frame_791
 C      -3.845663     1.076381    -3.022579      60.40
 H      -3.940950     0.195841    -3.455205      22.72
 C      -3.721179     1.998271    -0.781064      47.61
 H      -3.664320     1.820048     0.245288      15.32
 C      -3.633150     3.241961    -1.374651      40.56
 O      -3.127360     4.393701    -0.827670     220.21
 C      -3.226037     4.305150     0.640989     101.60
 H      -3.170389     5.381678     1.251479      21.32
 H      -2.694533     3.583823     1.178529      28.77
 H      -4.178788     4.220477     0.838344      28.95
 C      -3.737902     3.380177    -2.798836      10.47
 O      -3.502401     4.580036    -3.375439     104.80
 H      -3.579445     5.337751    -2.746627      29.57
 C      -3.798280     2.309554    -3.649227      67.58
 H      -3.828271     2.525638    -4.616450      22.08
 C      -3.904326     0.834793    -1.646970      34.18
 C      -4.246822    -0.529497    -1.089543      81.93
 H      -4.938493    -0.867729    -1.901127      24.91
 O      -4.928061    -0.483749     0.260201     189.00
 H      -4.201434    -0.215391     0.917007      21.30
 C      -2.865773    -1.500096    -0.931870      82.35
 H      -2.500055    -1.462288    -1.846416      25.13
 C      -3.214000    -2.965812    -0.417963      94.44
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 O      -4.060579    -3.747644    -1.164374     313.89
 H      -3.557712    -3.910060    -2.048772      27.45
 H      -3.681269    -2.809485     0.456988      25.88
 H      -2.049534    -3.415025    -0.252807      21.53
 C       1.569668    -1.134349    -1.490069      11.84
 H       2.024437    -1.676488    -2.339793      20.00
 C       1.272526     0.630197     0.232713      70.83
 H       1.609163     1.567464     0.575017      17.19
 C       0.046847     0.184271     0.518049       7.42
 O      -0.886204     0.802077     1.432881     180.07
 C      -0.218753     1.900181     2.369545     122.40
 H      -0.094372     2.708450     1.926718      27.38
 H      -1.021468     2.177886     3.086408      24.34
 H       0.397054     1.241997     2.761447      26.97
 C      -0.592061    -0.792008    -0.302182      -6.03
 O      -1.948938    -1.015387     0.101076     165.78
 C       0.245673    -1.452924    -1.309894      53.89
 H      -0.329305    -2.244926    -2.060446      17.72
 C       2.155827    -0.132103    -0.762284      52.58
 C       3.668420     0.084475    -0.775063     100.14
 H       4.433076    -0.443104    -1.418262      25.58
 O       3.942841     1.504281    -0.771653     230.82
 H       4.218387     1.748056     0.140750      27.55
 C       4.499422    -0.553077     0.454682      76.30
 H       4.020074    -0.008958     1.429387      23.54
 O       4.162748    -1.995312     0.453714     220.70
 H       4.176923    -2.122052    -0.566581      27.30
 C       6.073761    -0.434835     0.457807      97.04
 O       6.901503     0.696172     0.677737     263.58
 H       6.915224     0.795158     1.679064      27.48
 H       6.414950    -0.699325    -0.630819      28.26
 H       6.160896    -1.357222     1.005036      28.23
55
name= lig-ACN-Water-frame_792
 C      -3.863828     0.882933    -3.078280      44.38
 H      -3.716312     0.189233    -3.845898      21.06
 C      -3.644846     1.934574    -0.863055      64.56
 H      -3.462329     1.960540     0.271906      19.92
 C      -3.616872     3.210115    -1.535397      10.15
 O      -3.189100     4.339573    -0.870633     132.57
 C      -3.210569     4.307356     0.765249      62.39
 H      -2.550666     5.338034     0.753014      21.44
 H      -2.494259     3.657640     0.957817      29.77
 H      -4.081682     4.029596     1.140786      27.47
 C      -3.751586     3.370196    -2.909727      39.67
 O      -3.525972     4.632284    -3.500475     120.95
 H      -3.681840     5.334745    -2.721961      23.44
 C      -3.774531     2.229378    -3.688002      53.29
 H      -3.752549     2.208767    -4.716131      23.91
 C      -4.034931     0.875964    -1.627223      25.38
 C      -4.245221    -0.557287    -1.000354     108.29
 H      -4.844479    -1.284786    -1.521174      24.88
 O      -4.900678    -0.571694     0.271280     215.58
 H      -4.383991     0.027728     0.958048      22.08
 C      -2.962544    -1.415920    -0.889330      85.06
 H      -2.505191    -1.451211    -1.776689      26.78
 C      -3.101986    -2.881908    -0.373008      82.46
 O      -4.146328    -3.845428    -1.192122     251.35
 H      -4.057560    -3.678196    -2.073435      31.54
 H      -3.518516    -2.929108     0.597383      25.46
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 H      -2.051910    -3.502459    -0.220543      23.30
 C       1.563179    -1.099419    -1.444990      43.85
 H       2.147339    -1.566488    -2.217203      22.48
 C       1.471124     0.607689     0.210531      57.60
 H       2.019932     1.305156     0.815549      20.38
 C      -0.039178     0.224826     0.502610     -22.29
 O      -0.846561     0.777896     1.461120     177.09
 C      -0.220640     1.844021     2.325970     119.47
 H       0.306517     2.485588     1.861832      28.43
 H      -1.149367     2.126943     2.875352      23.78
 H       0.579951     1.624192     3.006087      27.11
 C      -0.599287    -0.927792    -0.252999      10.61
 O      -1.905900    -0.989122     0.017555     199.06
 C       0.157592    -1.451812    -1.281239      72.35
 H      -0.183293    -2.251922    -2.103527      20.16
 C       2.182160    -0.058388    -0.735402      32.17
 C       3.709428     0.083656    -0.808413      84.78
 H       3.800934    -0.310784    -1.893375      23.74
 O       4.050729     1.552726    -0.712022     197.86
 H       4.200602     1.709903     0.248155      26.45
 C       4.457610    -0.534697     0.435471      78.02
 H       3.964602    -0.300048     1.477852      23.88
 O       4.186989    -2.017733     0.465735     242.89
 H       4.589684    -2.561094    -0.247396      31.24
 C       5.997986    -0.483642     0.309342     103.13
 O       6.784829     0.636572     0.755399     270.15
 H       6.784418     0.866596     1.779888      25.58
 H       6.167572    -0.640745    -0.810240      28.00
 H       6.557117    -1.197815     0.834565      27.54
55
name= lig-ACN-Water-frame_793
 C      -3.939989     0.838636    -3.111866      72.85
 H      -4.102616    -0.177950    -3.554660      24.56
 C      -3.696517     1.946307    -0.996912      49.89
 H      -3.543087     1.797058     0.195328      21.77
 C      -3.513234     3.187856    -1.547892      -5.85
 O      -3.288313     4.347664    -0.751692     187.59
 C      -3.055015     4.310715     0.651985     105.53
 H      -2.836401     5.421414     1.102015      21.52
 H      -2.428945     3.624883     0.960620      31.65
 H      -3.927661     4.283413     1.197118      25.56
 C      -3.694799     3.341070    -3.024244     -26.09
 O      -3.579758     4.708801    -3.628109      51.94
 H      -3.742955     5.387955    -2.936572      24.05
 C      -3.779370     2.041089    -3.768449      31.03
 H      -3.587214     2.189236    -4.860750      16.23
 C      -4.043644     0.675659    -1.710347      12.24
 C      -4.190722    -0.648873    -0.882353     104.50
 H      -4.830925    -1.120353    -1.573013      28.15
 O      -4.938275    -0.594420     0.338208     200.99
 H      -4.373521    -0.219056     1.093829      24.68
 C      -2.914686    -1.525742    -0.962877      76.64
 H      -2.719121    -1.517672    -1.960368      26.86
 C      -3.231166    -2.969639    -0.426234      96.34
 O      -4.150099    -3.797516    -1.090097     281.89
 H      -3.823436    -3.733725    -2.047366      28.79
 H      -3.347032    -2.865317     0.675006      25.49
 H      -2.144918    -3.405154    -0.715567      21.60
 C       1.510608    -1.094660    -1.486500      62.10
 H       2.118685    -1.653894    -2.138804      25.57
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 C       1.389263     0.576399     0.356621      70.18
 H       1.754120     1.209152     1.184724      21.23
 C       0.159121     0.243146     0.434110      18.42
 O      -0.702468     0.789247     1.475620     214.90
 C      -0.220550     1.821421     2.296766     131.46
 H       0.182009     2.414788     1.667047      29.65
 H      -1.025879     2.604261     2.598570      25.30
 H       0.245310     1.270290     3.073113      26.91
 C      -0.538474    -0.791989    -0.227496     -11.33
 O      -1.964166    -0.926894     0.015004     101.85
 C       0.172756    -1.491827    -1.289224      58.57
 H      -0.442340    -2.261022    -1.831035      23.01
 C       2.191939    -0.099426    -0.661095      -0.47
 C       3.685106     0.195496    -0.786484      93.55
 H       4.233496     0.036068    -1.750976      21.90
 O       4.175750     1.581358    -0.657699     225.94
 H       4.171013     1.945026     0.275974      25.35
 C       4.418771    -0.713857     0.323694     101.14
 H       4.171247    -0.096897     1.216626      24.10
 O       4.173626    -2.061217     0.495532     256.37
 H       4.915471    -2.345543    -0.031024      30.03
 C       6.016321    -0.582164     0.207341      80.99
 O       6.681352     0.690342     0.789382     262.39
 H       6.360903     0.778759     1.732369      29.60
 H       6.348612    -0.464218    -0.869174      26.18
 H       6.181745    -1.549737     0.550963      28.62
55
name= lig-ACN-Water-frame_794
 C      -4.075979     0.720748    -3.121215      30.41
 H      -4.383824    -0.074021    -3.943478      22.50
 C      -3.784200     1.841022    -1.041226      55.03
 H      -3.855900     1.843493     0.168936      21.20
 C      -3.487752     3.205604    -1.622061       8.06
 O      -3.384879     4.378131    -0.787535     169.69
 C      -2.982371     4.321033     0.652974      90.66
 H      -2.463013     5.362492     0.761009      23.14
 H      -2.201550     3.662262     0.809045      30.12
 H      -3.803839     3.965087     1.195564      26.59
 C      -3.562317     3.337910    -3.039131      21.81
 O      -3.644589     4.577253    -3.716274     163.81
 H      -3.819588     5.230050    -3.067491      29.67
 C      -3.767454     2.093466    -3.783307      18.05
 H      -3.940550     2.054544    -4.964008      19.11
 C      -3.910819     0.672997    -1.680765      31.85
 C      -4.236427    -0.708185    -0.998382      76.45
 H      -4.942254    -1.282461    -1.454393      25.26
 O      -4.956433    -0.594145     0.432234     165.41
 H      -4.350319    -0.417433     1.131266      26.83
 C      -2.932168    -1.605843    -0.952200      82.30
 H      -2.342747    -1.614024    -1.807915      24.90
 C      -3.099643    -3.048650    -0.453900      95.28
 O      -4.236371    -3.720197    -1.043414     227.58
 H      -3.879614    -4.330726    -1.881989      27.13
 H      -3.535732    -3.044475     0.635589      23.38
 H      -2.126756    -3.729064    -0.357951      23.40
 C       1.537886    -1.080650    -1.475953      57.98
 H       2.011239    -1.578988    -2.291096      23.33
 C       1.540056     0.516239     0.418828      56.64
 H       2.154848     1.308250     0.984107      19.18
 C       0.049386     0.219417     0.550069       7.63
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 O      -0.676369     0.764176     1.439507     163.70
 C      -0.160696     1.930719     2.263869     111.84
 H       0.590002     2.496537     2.055457      28.36
 H      -1.248018     2.174850     2.589702      22.65
 H       0.308952     1.670978     3.264829      26.22
 C      -0.625992    -0.667130    -0.368727       4.88
 O      -1.951124    -0.872599    -0.006101     156.49
 C       0.191505    -1.467990    -1.216252      64.59
 H      -0.168961    -2.234582    -1.801288      24.29
 C       2.172281    -0.109732    -0.651106      18.89
 C       3.724726     0.217665    -0.780274      83.28
 H       3.878650    -0.264901    -1.743697      23.93
 O       4.218332     1.619861    -0.584988     231.75
 H       4.265046     1.698141     0.416430      25.37
 C       4.552581    -0.643694     0.281024      75.10
 H       4.241871    -0.400357     1.292901      24.96
 O       4.109431    -2.163982     0.470275     220.94
 H       4.641669    -2.927671     0.092545      29.77
 C       6.073104    -0.526928     0.153444     118.72
 O       6.516015     0.608771     0.768738     311.67
 H       6.449449     0.665659     1.704936      33.25
 H       6.422611    -0.518533    -0.888957      28.56
 H       6.739767    -1.199536     0.591546      27.86
55
name= lig-ACN-Water-frame_795
 C      -4.071867     0.873295    -3.180438      56.93
 H      -4.351765    -0.088074    -3.865958      23.12
 C      -3.767675     1.944162    -0.965001      39.24
 H      -4.032578     1.952411     0.161162      21.38
 C      -3.538736     3.130118    -1.587640      15.57
 O      -3.442333     4.340883    -0.935375     159.69
 C      -2.906612     4.273252     0.589777     100.87
 H      -2.650834     5.326694     0.900280      25.33
 H      -2.099378     3.604028     0.450413      26.37
 H      -3.602069     4.114651     1.433661      24.24
 C      -3.504803     3.194583    -3.033489      28.70
 O      -3.670062     4.384508    -3.766131     140.84
 H      -3.858657     5.139578    -3.085767      24.88
 C      -3.858898     2.059507    -3.686588      49.69
 H      -4.167289     2.343312    -4.812147      23.16
 C      -3.950159     0.607587    -1.790483       0.03
 C      -4.283808    -0.772759    -0.992578      84.01
 H      -4.939857    -1.258694    -1.591233      26.59
 O      -4.900064    -0.613462     0.373751     202.64
 H      -4.245011    -0.223700     1.011073      24.40
 C      -2.848890    -1.606229    -0.904212      90.76
 H      -2.681505    -1.639168    -1.990690      23.27
 C      -3.019954    -3.096127    -0.314162      77.94
 O      -4.343561    -3.710013    -1.056545     205.68
 H      -3.924243    -4.251809    -1.805554      29.41
 H      -3.228297    -2.894372     0.871721      23.61
 H      -2.081934    -3.732908    -0.464852      23.12
 C       1.592646    -1.050133    -1.426464      43.30
 H       2.187957    -1.479577    -2.247526      22.77
 C       1.501621     0.410795     0.378662      72.04
 H       1.921387     1.205963     1.111090      20.58
 C       0.181562     0.195278     0.502694      -8.45
 O      -0.737526     0.899216     1.566066     147.12
 C      -0.182495     1.977518     2.354017     116.75
 H       0.306972     2.477556     1.620559      26.95
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 H      -0.910549     2.927318     2.559289      23.45
 H       0.237901     1.436155     3.210956      25.60
 C      -0.630834    -0.603975    -0.376827     -15.08
 O      -1.993793    -0.853871    -0.037047     154.61
 C       0.202316    -1.405708    -1.256385      58.54
 H      -0.173794    -2.123878    -1.836025      24.20
 C       2.291394    -0.090513    -0.651753      40.53
 C       3.764327     0.077738    -0.782893      89.49
 H       4.156822     0.204493    -1.731488      25.54
 O       4.155852     1.572989    -0.542780     147.17
 H       4.545890     1.798331     0.322181      26.40
 C       4.620147    -0.778836     0.324542      80.32
 H       4.415045    -0.293288     1.233318      27.61
 O       4.029708    -2.185933     0.416029     217.47
 H       4.574489    -2.627235    -0.301833      30.13
 C       6.173037    -0.607686     0.106886     107.65
 O       6.437915     0.723786     0.769793     230.48
 H       6.609354     0.461563     1.730648      29.08
 H       6.348588    -0.414548    -0.918241      30.21
 H       6.494565    -1.530953     0.475436      29.89
55
name= lig-ACN-Water-frame_796
 C      -4.047975     0.768708    -3.118042      50.91
 H      -4.314104    -0.181563    -3.808134      22.67
 C      -3.791943     1.782853    -0.950545      74.69
 H      -3.807616     1.732204     0.124839      21.80
 C      -3.571716     3.079514    -1.562269      22.72
 O      -3.428277     4.292424    -0.898294     199.89
 C      -2.860445     4.264980     0.377637     121.88
 H      -2.569401     5.236584     0.515867      25.46
 H      -1.918155     3.645956     0.578176      26.86
 H      -3.702241     3.733281     0.930387      23.56
 C      -3.595583     3.144688    -2.960437      28.64
 O      -3.629211     4.259704    -3.746418     177.27
 H      -3.725386     5.090408    -3.131152      22.55
 C      -3.973874     2.063466    -3.809757      26.48
 H      -4.065559     2.202842    -4.961449      24.13
 C      -4.075552     0.714663    -1.659001      39.27
 C      -4.192426    -0.761506    -0.979906     109.90
 H      -4.870842    -1.387826    -1.489120      24.00
 O      -4.818433    -0.624661     0.239946     215.35
 H      -4.209310    -0.084490     0.903120      22.95
 C      -2.927038    -1.636350    -0.901649      78.31
 H      -2.324849    -1.748125    -1.886015      21.46
 C      -3.159506    -3.057139    -0.333753     101.25
 O      -4.266960    -3.662820    -0.947839     308.62
 H      -3.969587    -3.685196    -1.799597      35.35
 H      -3.239480    -3.268722     0.902481      23.90
 H      -2.313767    -3.669371    -0.619432      24.48
 C       1.626488    -1.055226    -1.464060      51.10
 H       2.120317    -1.763129    -2.200030      22.37
 C       1.485229     0.485649     0.420263      44.89
 H       2.046170     1.042422     1.259201      19.47
 C       0.004365     0.322052     0.588219      -3.42
 O      -0.781634     0.947890     1.586187     182.95
 C      -0.125654     2.065820     2.328755     108.90
 H       0.710351     2.567248     1.931150      24.22
 H      -1.074493     2.682683     2.778268      22.83
 H       0.551920     1.862892     3.284177      24.46
 C      -0.564063    -0.689517    -0.279490      -3.42
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 O      -1.949837    -0.804787    -0.086576     161.65
 C       0.230391    -1.275566    -1.361426      64.14
 H      -0.313727    -1.911576    -1.995283      20.69
 C       2.329718    -0.179930    -0.637978      13.36
 C       3.905485     0.089687    -0.724838      97.14
 H       4.101600    -0.470836    -1.546704      29.12
 O       4.064035     1.499296    -0.566296     200.80
 H       4.292480     1.554995     0.396311      23.45
 C       4.561513    -0.868420     0.310392      95.91
 H       4.343233    -0.567423     1.284372      27.23
 O       4.062230    -2.153944     0.303567     283.43
 H       3.935346    -2.544498    -0.581797      30.85
 C       6.124534    -0.681740     0.123048      94.44
 O       6.460829     0.767106     0.769048     211.03
 H       6.730327     0.854262     1.768212      26.90
 H       6.562995    -0.522458    -0.829308      29.83
 H       6.902096    -1.340108     0.520507      28.85
55
name= lig-ACN-Water-frame_797
 C      -4.123852     0.679903    -3.090583      40.43
 H      -4.174236    -0.309425    -3.648341      23.19
 C      -3.800659     1.778460    -0.822919      50.20
 H      -3.491631     1.716151     0.140761      21.15
 C      -3.634057     2.988867    -1.567411       3.58
 O      -3.380690     4.223750    -0.993925     201.20
 C      -2.802648     4.231205     0.364920     124.58
 H      -2.719999     5.177769     0.673038      27.52
 H      -1.824074     3.639386     0.126181      25.68
 H      -3.389742     3.896589     1.312839      24.99
 C      -3.840968     3.062470    -3.022697       1.71
 O      -3.534343     4.313709    -3.691393     141.42
 H      -3.496630     5.019114    -3.080196      27.54
 C      -4.002351     1.870265    -3.764587      61.94
 H      -3.929457     1.899447    -4.826089      21.60
 C      -4.112038     0.590528    -1.721968      23.07
 C      -4.140399    -0.713741    -1.101535     116.28
 H      -4.826170    -1.259955    -1.774724      28.45
 O      -4.791427    -0.617735     0.264001     116.07
 H      -4.154116    -0.329643     0.983575      24.67
 C      -2.859119    -1.566489    -0.889574      92.78
 H      -2.542744    -1.827584    -2.041600      21.60
 C      -3.134840    -3.009931    -0.321029      96.24
 O      -4.268605    -3.659057    -0.920186     235.76
 H      -4.443975    -3.414193    -1.899620      31.60
 H      -3.523068    -2.792708     0.867433      23.71
 H      -2.202695    -3.513029    -0.399952      26.43
 C       1.627858    -1.088499    -1.507476      51.39
 H       2.226503    -1.544896    -2.380478      20.40
 C       1.436488     0.535960     0.441298      70.94
 H       2.048741     1.226662     1.067913      20.17
 C       0.064076     0.366590     0.609846      -0.39
 O      -0.734325     1.012463     1.568745     173.95
 C      -0.037270     2.134690     2.355100      93.95
 H       0.333038     2.930956     1.614342      22.21
 H      -1.029373     2.706210     2.763870      22.38
 H       0.346537     1.444400     3.146254      22.51
 C      -0.543238    -0.670283    -0.218192      -1.53
 O      -1.921627    -0.795038    -0.105534     168.28
 C       0.188095    -1.166679    -1.372476      63.37
 H      -0.245883    -1.790254    -2.215018      21.79
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 C       2.205440    -0.217416    -0.508825      18.76
 C       3.747360    -0.008029    -0.667595      91.24
 H       4.172846    -0.016544    -1.595814      25.04
 O       4.047896     1.422978    -0.630616     211.03
 H       4.116831     1.867644     0.262372      25.83
 C       4.622751    -0.790740     0.404133      78.71
 H       4.339958    -0.542648     1.383278      26.44
 O       4.126251    -2.258068     0.134452     256.48
 H       3.409979    -2.137316    -0.553328      26.21
 C       6.172817    -0.579316     0.292554     101.13
 O       6.497256     0.728412     0.697622     324.60
 H       6.519484     0.630344     1.657670      30.67
 H       6.240330    -0.738877    -0.776641      29.34
 H       6.589175    -1.419918     0.985597      27.59
55
name= lig-ACN-Water-frame_798
 C      -4.228473     0.554505    -3.108455      57.30
 H      -4.254614    -0.349852    -3.659038      23.87
 C      -3.805427     1.749496    -0.929218      93.63
 H      -3.673321     1.652867     0.096694      24.11
 C      -3.785494     2.927617    -1.621991       9.45
 O      -3.362502     4.152930    -1.087728     148.98
 C      -2.684975     4.232487     0.408419      89.90
 H      -2.571947     5.194610     0.429184      26.38
 H      -1.550373     3.788870     0.425685      26.30
 H      -3.407766     3.548675     1.073568      22.76
 C      -3.963123     3.048805    -3.037552      10.39
 O      -3.475860     4.300634    -3.614788     149.16
 H      -3.414906     4.832418    -2.787988      23.38
 C      -4.010037     1.796213    -3.752227      28.77
 H      -3.964209     1.846234    -4.747917      21.31
 C      -3.987397     0.596224    -1.623533       0.14
 C      -4.181598    -0.781267    -1.009665      94.28
 H      -4.891275    -1.512583    -1.574942      24.76
 O      -4.806221    -0.642091     0.281701     164.54
 H      -4.101809    -0.396945     0.853876      28.84
 C      -2.772700    -1.530655    -1.010175      74.55
 H      -2.181730    -1.435010    -2.112346      20.65
 C      -3.069652    -2.859783    -0.252865      82.99
 O      -4.328987    -3.694360    -0.923874     110.38
 H      -4.224365    -3.252174    -1.935423      26.58
 H      -3.430543    -2.588327     0.922655      23.69
 H      -2.348595    -3.567734    -0.147805      27.11
 C       1.498158    -0.988820    -1.411344      47.81
 H       2.094075    -1.230878    -2.330216      22.96
 C       1.464433     0.561078     0.444991      61.03
 H       1.869382     1.428925     0.962017      23.44
 C       0.131594     0.298599     0.619325       5.63
 O      -0.659366     1.099145     1.503748     202.15
 C      -0.111687     2.107703     2.343659     117.41
 H       0.633120     2.748303     1.674025      25.43
 H      -0.870698     2.723577     2.993381      24.99
 H       0.902950     2.027909     2.994696      24.93
 C      -0.546609    -0.562352    -0.307966     -21.07
 O      -1.928122    -0.781169    -0.050903     145.69
 C       0.159800    -1.171814    -1.372018      64.62
 H      -0.633079    -1.712871    -2.082623      18.56
 C       2.184268    -0.246180    -0.489204      30.44
 C       3.633784     0.023930    -0.585530      96.14
 H       3.717494    -0.612105    -1.413984      27.61
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 O       4.035637     1.455351    -0.685655     225.51
 H       4.100935     1.699975     0.276826      27.13
 C       4.528052    -0.832702     0.459579      87.34
 H       4.177233    -0.576810     1.425662      28.30
 O       4.266460    -2.282496     0.035886     204.38
 H       3.384962    -2.135465    -0.472698      28.66
 C       6.084500    -0.634276     0.383658     101.77
 O       6.579891     0.724880     0.676000     276.90
 H       6.585683     1.054785     1.588801      29.73
 H       6.746888    -0.883809    -0.489040      27.24
 H       6.612050    -1.382253     1.154088      27.01
55
name= lig-ACN-Water-frame_799
 C      -4.191154     0.573267    -3.042756      67.57
 H      -4.381134    -0.252586    -3.606430      26.90
 C      -3.826791     1.669644    -1.004938      30.37
 H      -3.843262     1.853042     0.117866      22.54
 C      -3.871865     3.003965    -1.646527       4.21
 O      -3.282725     4.105008    -1.016434     267.37
 C      -2.655073     4.219865     0.229440     114.01
 H      -2.720528     5.122436     0.616743      24.53
 H      -1.556815     3.661789     0.327306      25.66
 H      -3.411645     3.843022     1.147998      20.98
 C      -3.886279     3.014246    -3.046921       6.23
 O      -3.499708     4.190003    -3.537093     156.67
 H      -3.301493     4.911495    -2.797772      18.73
 C      -4.105092     1.830427    -3.818075      75.82
 H      -4.071601     1.816821    -4.842221      26.34
 C      -4.028525     0.461523    -1.713420      40.56
 C      -4.152851    -0.811934    -0.930283     105.30
 H      -4.931572    -1.423626    -1.608459      23.69
 O      -4.801315    -0.707422     0.340598     154.79
 H      -4.400626    -0.144853     1.076061      22.87
 C      -2.807101    -1.517892    -0.934241      82.32
 H      -2.381873    -1.699297    -2.134524      20.22
 C      -3.119774    -2.890617    -0.308973     106.87
 O      -4.237062    -3.595158    -0.872974     224.97
 H      -3.968877    -3.843367    -1.812927      30.93
 H      -3.553986    -2.511486     0.773893      23.33
 H      -2.283725    -3.453457    -0.251789      27.39
 C       1.456974    -0.910780    -1.423930      62.20
 H       1.949471    -1.502485    -2.203436      21.79
 C       1.495657     0.574274     0.507036      69.19
 H       2.100661     1.254461     1.129634      20.99
 C       0.077741     0.348508     0.638813      15.03
 O      -0.667766     1.094577     1.461318     169.51
 C       0.022424     2.160710     2.280225     102.71
 H      -0.060209     3.256981     1.673162      20.12
 H      -0.940391     2.280284     2.894381      23.96
 H       0.622863     1.495648     3.001289      23.61
 C      -0.651702    -0.486318    -0.320231      20.89
 O      -1.926237    -0.737959     0.016765     172.63
 C       0.002502    -1.177255    -1.322652      72.16
 H      -0.220750    -1.944839    -2.259796      18.27
 C       2.180067    -0.116383    -0.436411      37.59
 C       3.728678    -0.001317    -0.628232      93.17
 H       4.233763    -0.149706    -1.579024      24.95
 O       3.989768     1.431511    -0.708477     226.93
 H       4.319342     1.827331     0.127093      29.01
 C       4.413010    -0.892846     0.428987     105.36
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 H       4.066355    -0.934736     1.426177      27.34
 O       4.426144    -2.228174     0.001310     254.32
 H       3.656628    -2.774683    -0.156595      30.09
 C       6.047950    -0.704205     0.510705      75.23
 O       6.663180     0.755318     0.666443     213.69
 H       6.640803     0.795798     1.711283      25.95
 H       6.230733    -1.077436    -0.540692      28.17
 H       6.375097    -1.319324     1.509930      25.96
55
name= lig-ACN-Water-frame_800
 C      -4.164122     0.639047    -3.214581      68.87
 H      -4.165350    -0.285813    -3.808485      23.92
 C      -3.934886     1.717105    -0.949845      60.38
 H      -3.633307     1.413818     0.177732      19.46
 C      -3.765615     2.862302    -1.548391      20.50
 O      -3.290894     4.134008    -1.076793     248.40
 C      -2.684632     4.182644     0.239773     112.78
 H      -2.385733     5.129166     0.239028      25.27
 H      -1.581715     3.680213     0.005934      27.47
 H      -3.222108     3.488185     1.101356      22.73
 C      -3.783631     2.966388    -2.999513       0.09
 O      -3.511590     4.192203    -3.622617     154.68
 H      -3.418370     4.760612    -2.770097      19.27
 C      -4.193864     1.854466    -3.769240      54.52
 H      -4.194382     1.939787    -4.898581      25.17
 C      -4.136898     0.530486    -1.690151      35.02
 C      -4.173883    -0.784962    -0.966490      98.65
 H      -4.808072    -1.637051    -1.537279      21.74
 O      -4.827105    -0.775222     0.434352      93.30
 H      -4.198964    -0.116924     0.931989      24.93
 C      -2.899877    -1.535951    -0.747521      76.15
 H      -2.355862    -1.504796    -1.920660      19.02
 C      -3.057244    -2.946357    -0.231038     109.72
 O      -4.165187    -3.542734    -0.915422     280.83
 H      -3.799049    -4.244434    -1.360325      32.42
 H      -3.303510    -2.970346     0.960119      23.90
 H      -2.206156    -3.510390    -0.341609      26.79
 C       1.436354    -0.916429    -1.417472      45.84
 H       2.043032    -1.438690    -2.102382      24.47
 C       1.473595     0.543827     0.578222      76.99
 H       1.864885     1.129155     1.447601      18.30
 C       0.104659     0.456042     0.528716       8.57
 O      -0.733008     1.127796     1.468659     220.58
 C      -0.113378     2.109422     2.299130     109.46
 H       0.493558     3.037637     1.629696      22.02
 H      -0.705047     2.423485     3.188468      24.92
 H       1.075689     1.991049     2.627881      22.11
 C      -0.658248    -0.493160    -0.271436     -13.78
 O      -2.061372    -0.725075     0.066066     146.47
 C       0.092572    -1.117011    -1.297349      63.92
 H      -0.632149    -1.908981    -1.840901      17.36
 C       2.209919    -0.113230    -0.615498      15.26
 C       3.760415     0.015957    -0.708832      81.18
 H       3.995391    -0.551988    -1.650279      25.98
 O       3.995049     1.481355    -0.680561     181.23
 H       4.267700     1.743280     0.253881      25.39
 C       4.473274    -0.849665     0.467512      88.23
 H       3.756299    -0.657778     1.191765      27.07
 O       4.594628    -2.315080    -0.047658     223.88
 H       3.711105    -2.488096     0.326846      29.59
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 C       5.966099    -0.599801     0.612793     102.64
 O       6.655090     0.628424     0.664815     245.22
 H       6.888055     1.005840     1.638195      25.31
 H       6.553827    -1.086576    -0.236031      26.75
 H       6.428550    -1.438869     1.437390      25.47
55
name= lig-ACN-Water-frame_801
 C      -4.210719     0.570724    -3.160213      60.63
 H      -4.120682    -0.366396    -3.836058      22.20
 C      -4.010876     1.636938    -0.826212      42.37
 H      -3.774628     1.585027     0.385310      14.62
 C      -3.555632     2.904833    -1.613408      28.36
 O      -3.394155     4.146371    -1.119689     192.81
 C      -2.557371     4.143819     0.222029      98.81
 H      -2.532632     5.091662     0.654285      26.22
 H      -1.578539     3.388310     0.272311      21.76
 H      -3.393011     3.906456     1.058223      24.03
 C      -3.786303     2.997874    -2.987841      17.08
 O      -3.529466     4.197386    -3.678529     187.95
 H      -3.529260     4.978287    -3.183801      28.43
 C      -4.159342     1.935466    -3.776742      48.03
 H      -4.239205     2.241644    -4.937960      23.10
 C      -4.231130     0.559505    -1.749212      26.37
 C      -4.332365    -0.836801    -0.915422     107.66
 H      -5.090165    -1.495139    -1.537899      25.04
 O      -4.826379    -0.775069     0.419143     166.33
 H      -4.252227    -0.572202     1.187914      24.26
 C      -2.882326    -1.508422    -0.709784      73.55
 H      -2.340716    -1.771539    -1.811484      17.52
 C      -2.934852    -3.005014    -0.091461      88.01
 O      -4.149721    -3.592372    -0.950668     165.47
 H      -3.716735    -4.495814    -1.383663      27.07
 H      -3.086338    -3.032548     1.043648      24.76
 H      -2.057612    -3.514247    -0.422434      23.52
 C       1.518943    -0.973515    -1.490348      36.16
 H       1.800464    -1.378820    -2.412210      19.68
 C       1.490539     0.458199     0.431647      72.03
 H       2.178225     1.045946     1.105558      18.24
 C      -0.007946     0.517327     0.548805       6.80
 O      -0.782020     1.141789     1.495467     179.42
 C      -0.092380     2.143581     2.325529      79.48
 H      -0.240119     3.197619     1.527792      17.83
 H      -0.806409     2.400780     3.137295      23.35
 H       0.799122     1.513100     2.800476      21.02
 C      -0.688297    -0.482007    -0.196956      11.37
 O      -2.008919    -0.648128     0.156575     162.09
 C       0.034753    -1.131384    -1.225731      61.96
 H      -0.361237    -1.901100    -1.980711      18.29
 C       2.207619    -0.081511    -0.552724      28.82
 C       3.702681     0.026915    -0.738779      86.31
 H       4.066917    -0.240796    -1.793999      23.18
 O       4.061478     1.498043    -0.668860     207.57
 H       3.963774     1.742316     0.308522      23.12
 C       4.528197    -0.757760     0.350673      81.99
 H       4.237300    -0.856598     1.340088      24.00
 O       4.623107    -2.316838    -0.000072     196.65
 H       3.975762    -3.000081     0.348063      27.22
 C       6.061465    -0.642278     0.681770      79.11
 O       6.665570     0.621739     0.691709     320.06
 H       6.429175     1.066418     1.559661      27.48
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 H       6.387118    -1.183944    -0.251251      25.85
 H       6.148101    -1.170897     1.828594      24.51
55
name= lig-ACN-Water-frame_802
 C      -4.272117     0.684485    -3.055623      33.19
 H      -4.454116    -0.264238    -3.669563      23.27
 C      -3.946999     1.734396    -1.006497      55.86
 H      -4.326651     1.778014     0.117030      19.10
 C      -3.574032     2.862118    -1.582888      25.13
 O      -3.319429     4.216504    -0.942885     215.78
 C      -2.648220     4.160073     0.218129     115.16
 H      -2.064289     5.110800     0.297433      24.42
 H      -1.677742     3.412929     0.004743      24.63
 H      -3.237016     3.576195     1.036466      22.83
 C      -3.782041     3.040733    -3.045111       2.87
 O      -3.553396     4.222430    -3.754396      81.03
 H      -3.775568     4.862724    -3.021682      26.44
 C      -4.070984     1.842312    -3.755384      56.41
 H      -4.179666     1.781584    -4.965313      21.20
 C      -4.265237     0.462396    -1.614383      26.41
 C      -4.321643    -0.872299    -0.885320     104.33
 H      -4.945593    -1.653310    -1.413225      24.05
 O      -4.891937    -0.726136     0.448747     176.26
 H      -4.145903    -0.494077     0.982676      26.99
 C      -2.877479    -1.578370    -0.728180      68.31
 H      -2.388235    -1.461867    -1.823323      21.31
 C      -2.971758    -3.003303    -0.204026     114.92
 O      -4.021336    -3.655683    -0.829736     269.28
 H      -3.718300    -4.363116    -1.490817      28.89
 H      -3.281861    -2.951882     0.860614      25.57
 H      -1.977594    -3.525539    -0.124836      24.79
 C       1.377709    -0.970217    -1.504233      46.01
 H       1.956465    -1.340658    -2.314546      21.83
 C       1.381561     0.564127     0.415511      60.23
 H       1.873158     1.323487     1.081692      21.08
 C       0.054521     0.443385     0.617164      20.05
 O      -0.788807     1.143922     1.511637     177.30
 C      -0.203863     2.173374     2.363087     102.12
 H       0.386972     3.326324     1.997531      21.43
 H      -0.946394     2.252819     3.135826      24.27
 H       0.933960     1.881259     2.880201      22.46
 C      -0.642626    -0.480541    -0.213463       1.83
 O      -1.995132    -0.624947     0.183378     123.68
 C       0.082949    -1.202424    -1.219286      77.56
 H      -0.505757    -1.761405    -1.902802      22.25
 C       2.179984    -0.257848    -0.649754      16.81
 C       3.733063     0.113157    -0.696903      80.84
 H       4.063134    -0.210719    -1.757131      22.13
 O       4.122271     1.483119    -0.654191     243.56
 H       4.055971     1.977335     0.195573      25.94
 C       4.542866    -0.893920     0.338309      94.58
 H       3.835133    -0.524841     1.051319      23.83
 O       4.621440    -2.261546     0.019452     272.56
 H       3.853309    -2.566680     0.529550      29.90
 C       6.158309    -0.705180     0.602469      88.15
 O       6.694351     0.710535     0.693196     273.93
 H       6.570521     1.018781     1.625821      25.83
 H       6.933017    -1.384905     0.181835      26.77
 H       6.269030    -1.161721     1.822194      24.04
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name= lig-ACN-Water-frame_803
 C      -4.342959     0.595327    -2.950722      56.79
 H      -4.539767    -0.219395    -3.598278      26.01
 C      -3.964116     1.760827    -0.964779      24.19
 H      -3.976756     1.890747     0.153552      22.71
 C      -3.698316     3.097632    -1.709263       6.38
 O      -3.375053     4.175950    -0.968245     135.59
 C      -2.529859     4.089076     0.341392      97.57
 H      -2.326257     5.232064     0.505523      24.91
 H      -1.607129     3.314433     0.173968      23.81
 H      -3.042845     4.062132     1.312172      23.68
 C      -3.682508     3.031356    -3.093822      28.74
 O      -3.605909     4.254211    -3.758490     158.92
 H      -3.616525     5.138696    -3.174484      21.39
 C      -3.992007     1.783542    -3.682995      48.84
 H      -3.926471     1.673302    -4.841661      21.84
 C      -4.204511     0.521345    -1.591271      18.00
 C      -4.235766    -0.869039    -0.839100      97.48
 H      -4.845050    -1.535270    -1.433245      28.61
 O      -4.914664    -0.668452     0.480367     133.94
 H      -4.440787    -0.177685     1.222642      24.37
 C      -2.859077    -1.462794    -0.784793      92.57
 H      -2.464011    -1.500768    -1.881787      23.20
 C      -2.959570    -2.909445    -0.178716     104.55
 O      -3.952468    -3.829041    -0.762476     282.17
 H      -3.652313    -3.852366    -1.611423      35.03
 H      -3.260841    -2.696985     0.835721      26.45
 H      -1.956103    -3.498874    -0.235622      24.10
 C       1.421295    -1.012794    -1.526047      46.19
 H       1.741641    -1.678047    -2.348249      20.00
 C       1.477292     0.647222     0.368319      59.29
 H       2.009149     1.433856     0.905568      21.85
 C       0.059367     0.361932     0.659337       9.59
 O      -0.729110     1.176685     1.503538     158.38
 C      -0.238984     2.166551     2.503238      80.01
 H      -0.177464     3.115854     1.560870      19.38
 H      -1.012902     2.585398     3.217091      23.67
 H       0.735240     1.624250     3.074605      22.60
 C      -0.661377    -0.559799    -0.185493      10.26
 O      -2.022137    -0.732214     0.081446     208.63
 C      -0.078679    -1.266632    -1.257236      47.71
 H      -0.599041    -1.900757    -1.789341      22.08
 C       2.157944    -0.106855    -0.516578      21.09
 C       3.783205     0.019105    -0.776569      73.48
 H       4.011756    -0.340736    -1.838627      24.60
 O       4.141298     1.508281    -0.639033     199.21
 H       4.479325     1.428598     0.271975      24.65
 C       4.680523    -0.815106     0.347418      94.04
 H       4.455334    -0.911073     1.410493      23.02
 O       4.495133    -2.281952     0.037072     239.17
 H       3.644006    -2.669706     0.291396      28.90
 C       6.217995    -0.589955     0.641207      79.79
 O       6.693374     0.719214     0.649523     273.58
 H       6.963144     0.839285     1.637000      26.17
 H       6.652905    -1.068418    -0.265986      26.73
 H       6.387585    -1.176275     1.793971      24.81
55
name= lig-ACN-Water-frame_804
 C      -4.293706     0.548375    -2.997481      63.67
 H      -4.298643    -0.375751    -3.434377      23.26
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 C      -3.937580     1.900856    -0.865405      72.33
 H      -3.520142     1.877907     0.061824      22.71
 C      -3.815345     2.999787    -1.601127       6.89
 O      -3.431324     4.218690    -0.966596     104.17
 C      -2.465566     4.105933     0.418602      71.89
 H      -1.898064     5.228948     0.382947      22.95
 H      -1.669572     3.288266     0.422985      26.81
 H      -3.253965     3.776017     0.944295      25.64
 C      -3.688778     3.056794    -3.064887      10.47
 O      -3.626905     4.274053    -3.837100     150.15
 H      -3.463817     4.920382    -3.093080      20.30
 C      -3.939741     1.780189    -3.678468      32.16
 H      -3.922542     1.789604    -4.773186      23.34
 C      -4.156119     0.655045    -1.533083      -7.02
 C      -4.262213    -0.643561    -0.775366     103.38
 H      -4.871508    -1.283105    -1.324326      28.43
 O      -4.932024    -0.651943     0.470858     193.38
 H      -4.183445    -0.434931     1.191566      24.66
 C      -2.896174    -1.487116    -0.852814      71.60
 H      -2.534856    -1.500431    -1.897722      25.21
 C      -2.929324    -2.853174    -0.099763      94.77
 O      -3.864233    -3.962445    -0.754906     215.02
 H      -4.074160    -3.604899    -1.675166      30.03
 H      -3.135297    -2.796636     0.900568      27.81
 H      -1.782634    -3.165800    -0.173893      24.85
 C       1.372330    -1.030367    -1.318701      53.14
 H       2.068553    -1.473031    -2.080076      23.41
 C       1.469412     0.675854     0.409673      51.19
 H       1.985436     1.431608     0.948698      21.21
 C       0.100086     0.409599     0.652398       0.10
 O      -0.741693     1.126240     1.535423     166.03
 C      -0.264248     2.136664     2.464076      92.07
 H       0.344808     3.347705     2.200457      20.88
 H      -1.237730     2.109810     3.035593      23.05
 H       0.725918     1.801754     3.244476      22.95
 C      -0.668706    -0.645856    -0.149292      -5.61
 O      -2.007620    -0.763124     0.038749     158.38
 C       0.039657    -1.240185    -1.271684      77.29
 H      -0.292763    -1.920556    -1.834757      25.67
 C       2.211486    -0.137084    -0.695294      27.82
 C       3.784545    -0.022431    -0.702842      86.36
 H       4.189859    -0.362197    -1.683672      24.28
 O       4.144251     1.436515    -0.619030     179.68
 H       4.927175     1.707313    -0.076450      23.93
 C       4.637256    -0.777304     0.434915      74.80
 H       3.961399    -0.315370     1.240859      23.74
 O       4.430177    -2.307343     0.032455     213.13
 H       3.422878    -2.260033     0.109938      27.58
 C       6.232745    -0.595376     0.469501      89.77
 O       6.731335     0.796662     0.648374     258.60
 H       6.732899     1.200042     1.644991      24.82
 H       6.764461    -1.047147    -0.366364      27.55
 H       6.767739    -1.365815     1.385251      25.43
55
name= lig-ACN-Water-frame_805
 C      -4.076077     0.717575    -2.926877      69.19
 H      -4.204813    -0.215373    -3.399279      27.26
 C      -3.867604     1.873312    -0.776146      44.33
 H      -3.889375     1.787849     0.217980      26.13
 C      -3.739653     3.122743    -1.546153      -4.51
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 O      -3.380129     4.300563    -0.906403      81.39
 C      -2.609007     4.097203     0.300509     117.76
 H      -2.100541     5.275191     0.621144      24.18
 H      -1.878942     3.352984     0.005174      26.46
 H      -2.960384     4.064093     1.260804      27.51
 C      -3.862226     3.018599    -2.990405     -11.55
 O      -3.610377     4.186237    -3.824924     155.86
 H      -3.449220     5.002625    -3.412037      30.07
 C      -3.937411     1.799401    -3.750011      63.50
 H      -3.923890     1.765843    -4.764003      19.47
 C      -4.171674     0.723877    -1.540995      37.54
 C      -4.313990    -0.610524    -0.847815      99.73
 H      -5.020479    -1.055727    -1.453524      26.41
 O      -4.910839    -0.609161     0.510401     191.66
 H      -4.257670    -0.529021     1.283943      23.46
 C      -3.022136    -1.518553    -0.794848      60.78
 H      -2.635943    -1.589163    -1.748152      24.83
 C      -2.976507    -2.954261    -0.173111     110.02
 O      -3.697445    -3.959172    -0.696690     273.37
 H      -4.120242    -3.642139    -1.657888      28.34
 H      -3.322856    -2.788878     0.749540      26.86
 H      -1.857303    -3.388784    -0.080595      24.11
 C       1.602449    -1.090453    -1.311723      61.35
 H       1.892820    -1.804137    -2.134268      21.57
 C       1.467372     0.609133     0.370258      74.79
 H       1.895343     1.342133     0.988179      22.38
 C       0.092690     0.410036     0.566106      13.69
 O      -0.717949     1.064214     1.524405     167.05
 C      -0.276671     2.043723     2.524416      72.97
 H       0.058587     3.128112     1.752010      19.62
 H      -1.080409     2.590981     3.213086      22.40
 H       0.590793     1.362261     3.213715      21.69
 C      -0.570346    -0.583221    -0.166182       6.32
 O      -1.950972    -0.691003     0.086488     146.75
 C       0.134004    -1.258551    -1.165191      51.55
 H      -0.421035    -1.780522    -1.807162      20.12
 C       2.254388    -0.030268    -0.530212      31.44
 C       3.831620     0.031900    -0.677470      92.40
 H       4.111419    -0.483790    -1.607219      25.96
 O       4.127654     1.388193    -0.653386     219.15
 H       5.030324     1.336085    -0.215484      23.06
 C       4.508669    -0.821971     0.406743      76.14
 H       4.261825    -0.761250     1.600199      23.23
 O       4.357434    -2.180334     0.132024     241.79
 H       3.462811    -2.419091    -0.211472      29.59
 C       6.202714    -0.580819     0.299357      66.67
 O       6.745008     0.857597     0.647895     208.65
 H       6.357979     1.006075     1.555702      25.21
 H       6.527738    -0.698836    -0.697148      26.67
 H       6.557919    -1.360049     1.261057      24.48
55
name= lig-ACN-Water-frame_806
 C      -3.931717     0.698695    -2.904984      87.41
 H      -4.059621    -0.257591    -3.483308      24.93
 C      -3.876697     1.940077    -0.765697      72.70
 H      -4.131854     2.103005     0.238700      22.38
 C      -3.679332     3.121176    -1.520975      29.07
 O      -3.414162     4.385705    -0.926355     171.80
 C      -2.645415     4.168404     0.272429      99.94
 H      -1.984288     5.303440     0.320732      21.26
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 H      -1.886403     3.444543     0.171430      24.10
 H      -3.420945     3.806011     0.891552      21.78
 C      -3.913529     3.133980    -2.941948      16.30
 O      -3.593230     4.094658    -3.808037     168.58
 H      -3.760242     4.981926    -3.296652      26.19
 C      -3.970748     1.965376    -3.680954      38.82
 H      -3.830953     1.950904    -4.690898      23.82
 C      -4.069862     0.735797    -1.483798      18.18
 C      -4.369287    -0.742742    -0.810591      84.09
 H      -4.986984    -1.384370    -1.319771      23.31
 O      -4.927715    -0.546481     0.518916     239.83
 H      -4.259672    -0.092389     1.022823      24.60
 C      -2.941937    -1.473846    -0.768774      68.87
 H      -2.632220    -1.488735    -1.710383      20.95
 C      -2.956781    -2.890053    -0.060692      91.40
 O      -3.677943    -4.049288    -0.750417     323.45
 H      -3.715862    -3.898173    -1.703629      30.49
 H      -3.263355    -2.907927     0.878565      25.74
 H      -1.769410    -3.069602    -0.083656      22.00
 C       1.669015    -1.120736    -1.321318      31.39
 H       2.403432    -1.530407    -2.057093      18.66
 C       1.494246     0.680491     0.446667      56.21
 H       2.003818     1.410340     1.056294      21.77
 C       0.074167     0.454042     0.615899       2.50
 O      -0.758328     0.995615     1.529139     168.20
 C      -0.229928     1.924025     2.462788      78.58
 H       0.544838     2.879917     1.844875      19.90
 H      -1.299137     2.190106     2.935773      20.44
 H       0.734055     1.629388     3.340039      21.58
 C      -0.599634    -0.516447    -0.235636      -0.69
 O      -1.969201    -0.661174     0.096149     165.08
 C       0.295063    -1.316862    -1.108876      69.71
 H      -0.134548    -2.053774    -1.761083      23.81
 C       2.290738    -0.186039    -0.488196      21.18
 C       3.722100     0.034708    -0.641824      90.46
 H       3.963736    -0.370037    -1.612510      24.47
 O       4.204144     1.434959    -0.691529     232.15
 H       4.964992     1.662305    -0.132003      22.22
 C       4.601062    -0.759990     0.407563      81.85
 H       4.316652    -0.367069     1.559364      21.63
 O       4.285765    -2.180769     0.231521     232.84
 H       3.708848    -2.242330    -0.560389      28.62
 C       6.069420    -0.443777     0.252927     102.24
 O       6.637969     0.785978     0.626242     278.53
 H       6.581214     1.078319     1.516029      30.69
 H       6.353745    -0.675165    -0.769232      27.34
 H       6.822566    -1.411389     0.709888      25.26
55
name= lig-ACN-Water-frame_807
 C      -3.924281     0.698401    -2.907930      51.44
 H      -3.700699    -0.282797    -3.502374      21.61
 C      -3.987630     1.961443    -0.815670      43.18
 H      -3.899388     1.959351     0.327200      15.20
 C      -3.737822     3.155189    -1.528918      43.15
 O      -3.459594     4.396459    -1.036611     174.69
 C      -2.631245     4.272512     0.330437      93.18
 H      -2.283826     5.408294     0.942108      23.57
 H      -1.941510     3.536662     0.208857      25.67
 H      -3.233393     4.072877     1.264764      25.02
 C      -3.816856     3.150282    -2.918716       7.52
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 O      -3.590164     4.271802    -3.804624      96.12
 H      -3.786750     5.240071    -3.348301      23.07
 C      -3.980759     1.857601    -3.504899      54.03
 H      -4.000323     2.054213    -4.567958      23.81
 C      -3.980508     0.625595    -1.471018      39.30
 C      -4.249063    -0.701015    -0.727038     106.43
 H      -4.924285    -1.262982    -1.289892      26.34
 O      -4.964420    -0.499064     0.507435     223.24
 H      -4.466663     0.062774     1.160694      27.92
 C      -2.874817    -1.465933    -0.704748      97.32
 H      -2.537040    -1.607763    -1.617684      23.79
 C      -2.875440    -2.863573    -0.006822      92.09
 O      -3.644748    -4.057031    -0.805366     295.68
 H      -3.157347    -4.048866    -1.568227      32.06
 H      -3.355832    -2.779941     0.851238      26.15
 H      -1.805991    -3.328369     0.145834      22.16
 C       1.640209    -1.094143    -1.249125      57.74
 H       2.098768    -1.623813    -2.083908      20.90
 C       1.493422     0.638461     0.499641      56.69
 H       2.052142     1.398785     1.085640      19.41
 C       0.137387     0.409790     0.580763       5.09
 O      -0.769434     0.933057     1.545830     150.77
 C      -0.174016     1.888457     2.433603      76.16
 H       0.283436     3.012907     1.867620      19.64
 H      -0.989705     2.490205     3.152694      21.37
 H       0.403407     1.024786     3.250488      19.97
 C      -0.507059    -0.553823    -0.314231      -3.14
 O      -1.977580    -0.655978     0.040018     169.87
 C       0.251470    -1.398262    -1.121727      63.78
 H      -0.176777    -2.356057    -1.602762      18.02
 C       2.224221    -0.115373    -0.354380      25.34
 C       3.805733     0.080806    -0.625146      90.25
 H       4.071038    -0.333793    -1.565689      25.49
 O       4.224286     1.519160    -0.730801     224.65
 H       4.656479     1.642425     0.139828      22.71
 C       4.580936    -0.627541     0.464592      76.85
 H       4.030114    -0.262002     1.496263      20.71
 O       4.268774    -2.191904     0.329440     159.10
 H       4.109671    -2.208365    -0.684074      27.25
 C       6.093474    -0.496042     0.200078      84.61
 O       6.528152     0.820052     0.630007     248.51
 H       6.529105     0.738109     1.636182      27.96
 H       6.238893    -0.370839    -0.881622      27.22
 H       6.620353    -1.477455     0.845008      24.01
55
name= lig-ACN-Water-frame_808
 C      -3.915944     0.557274    -2.802234      46.68
 H      -3.939962    -0.410156    -3.497754      22.16
 C      -4.015378     1.882188    -0.858283      53.55
 H      -3.997715     1.880688     0.364143      19.78
 C      -3.820928     3.168268    -1.529391     -13.91
 O      -3.388848     4.401198    -0.870029     111.87
 C      -2.737337     4.397353     0.388674     108.26
 H      -2.336719     5.572486     0.181224      21.04
 H      -1.796560     3.922698     0.237263      30.06
 H      -3.439514     3.903224     1.174844      23.03
 C      -3.726387     3.182046    -3.015681      15.67
 O      -3.627333     4.396439    -3.747293     145.07
 H      -3.589870     5.202649    -3.028772      16.65
 C      -3.941120     1.921145    -3.607343      40.80
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 H      -4.070175     1.549151    -4.667325      25.82
 C      -3.977006     0.677748    -1.464094      52.30
 C      -4.098784    -0.625011    -0.699425      89.29
 H      -4.723000    -1.224477    -1.373407      25.65
 O      -5.002637    -0.473182     0.518561     188.13
 H      -4.450043    -0.206919     1.369862      23.38
 C      -2.811418    -1.560125    -0.664741      85.65
 H      -2.654111    -1.582542    -1.643935      25.87
 C      -2.917532    -3.006293    -0.005843     116.67
 O      -3.521401    -3.900858    -0.781220     288.36
 H      -2.998764    -4.214934    -1.660428      27.37
 H      -3.488065    -2.936347     0.832547      26.77
 H      -1.853461    -3.243011     0.375285      25.05
 C       1.554377    -1.089859    -1.172276      48.40
 H       2.238135    -1.646021    -1.780884      24.16
 C       1.493518     0.604768     0.585730      92.30
 H       1.805248     1.401265     1.334756      15.79
 C       0.064766     0.332899     0.574578      13.12
 O      -0.756389     0.922549     1.494921     177.57
 C      -0.176661     1.846182     2.500367      69.54
 H       0.682232     2.526268     1.781700      19.78
 H      -1.171061     2.292970     3.019951      21.22
 H       0.877920     1.523493     3.236299      21.21
 C      -0.571402    -0.639573    -0.228059      23.44
 O      -1.823324    -0.615796    -0.013847     160.01
 C       0.169962    -1.430345    -1.117624      63.75
 H      -0.414837    -2.257580    -1.818861      19.12
 C       2.320835    -0.044502    -0.460521      19.54
 C       3.763802     0.180936    -0.628858      94.86
 H       4.039365    -0.282807    -1.546194      26.57
 O       4.202320     1.545111    -0.725626     223.49
 H       4.428836     2.010068     0.140834      23.88
 C       4.536649    -0.714051     0.469056      88.22
 H       4.540836    -0.512276     1.630069      23.63
 O       4.255044    -2.060619     0.412876     255.34
 H       4.601150    -2.595240    -0.332704      30.19
 C       6.066041    -0.499576     0.264699      74.72
 O       6.481585     0.864368     0.712921     227.75
 H       6.516415     1.015177     1.761234      25.72
 H       6.299279    -0.782031    -0.791837      27.33
 H       6.816966    -1.426148     0.797323      26.41
55
name= lig-ACN-Water-frame_809
 C      -3.936410     0.713892    -2.944269      49.79
 H      -4.239088    -0.342095    -3.290769      24.32
 C      -3.948234     2.024645    -0.803970      28.80
 H      -4.233568     2.211122     0.406182      18.09
 C      -3.768751     3.140156    -1.560959      22.00
 O      -3.457995     4.325752    -0.863224     178.15
 C      -2.743124     4.510494     0.416912      99.09
 H      -2.781311     5.727184     0.874058      21.97
 H      -1.842544     3.997487     0.630128      27.32
 H      -3.381869     4.288768     1.384510      22.02
 C      -3.743805     3.162323    -2.985948      -3.40
 O      -3.659050     4.342632    -3.705076     126.02
 H      -3.648195     5.311589    -3.227306      19.70
 C      -3.847960     1.819484    -3.702150      45.90
 H      -3.800145     2.063205    -4.840201      18.86
 C      -3.976650     0.673331    -1.439766      -4.41
 C      -4.144744    -0.713163    -0.653569      90.60
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 H      -4.798324    -1.393698    -1.259594      25.77
 O      -4.947535    -0.472639     0.512460     201.71
 H      -4.399528    -0.575802     1.333314      25.21
 C      -2.775248    -1.509062    -0.620901      93.18
 H      -2.431726    -1.825370    -1.524880      24.99
 C      -2.882553    -2.921193     0.139354     106.30
 O      -3.481249    -3.892242    -0.842076     221.73
 H      -2.922357    -3.729194    -1.753175      26.41
 H      -3.498385    -2.971728     0.959909      27.11
 H      -1.856103    -3.289499     0.415413      25.68
 C       1.621042    -1.102687    -1.188374      67.93
 H       2.170992    -1.674228    -1.888743      22.76
 C       1.459216     0.546744     0.543607      90.19
 H       2.075268     1.185515     1.224611      19.51
 C       0.164301     0.294418     0.687952      22.24
 O      -0.753209     0.942730     1.541475     191.97
 C      -0.110353     1.833304     2.421972     106.93
 H       0.047684     2.997865     2.047977      21.20
 H      -1.091768     2.251828     3.093093      22.50
 H       0.263503     1.116852     3.444469      20.83
 C      -0.500086    -0.695298    -0.134275      21.62
 O      -1.924280    -0.658396    -0.015372     186.60
 C       0.238215    -1.383650    -1.097587      81.40
 H      -0.193196    -2.129905    -2.057737      18.05
 C       2.126935    -0.027192    -0.493861      34.09
 C       3.737875     0.147382    -0.595820      82.40
 H       4.024055    -0.202300    -1.563493      25.33
 O       4.174900     1.573270    -0.707966     221.61
 H       4.359627     1.819396     0.230950      26.90
 C       4.636927    -0.655894     0.496758      71.72
 H       4.061123    -0.150419     1.307975      24.12
 O       4.196755    -2.085569     0.481567     254.35
 H       4.909893    -2.434158    -0.063918      31.92
 C       6.120665    -0.433541     0.394663      95.62
 O       6.469105     0.865759     0.755906     278.95
 H       6.579135     0.937992     1.729053      28.67
 H       6.562765    -0.398826    -0.606090      26.79
 H       6.590601    -1.250364     1.289337      24.88
55
name= lig-ACN-Water-frame_810
 C      -4.010495     0.748418    -2.910927      52.32
 H      -3.988250    -0.093200    -3.609970      23.44
 C      -3.903562     1.919238    -0.785714      52.59
 H      -3.978809     2.024027     0.446400      16.67
 C      -3.612403     3.128740    -1.514497      24.84
 O      -3.553288     4.397834    -0.936473     145.58
 C      -2.846629     4.588030     0.590428      87.08
 H      -2.701762     5.721926     0.297964      23.17
 H      -1.830460     4.208966     0.313836      26.85
 H      -3.584809     3.972063     1.250633      22.73
 C      -3.762237     3.091342    -2.959460      29.73
 O      -3.686324     4.231120    -3.740605     177.54
 H      -3.528823     4.953308    -3.124139      26.69
 C      -3.742789     1.996663    -3.684988      55.78
 H      -3.684063     1.856360    -4.824375      22.69
 C      -4.012148     0.746097    -1.498091      33.08
 C      -4.242569    -0.727380    -0.791084      77.18
 H      -4.964464    -1.342503    -1.469430      26.12
 O      -4.852928    -0.527209     0.551092     185.21
 H      -4.208653    -0.376201     1.243338      25.46
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 C      -2.866509    -1.557106    -0.558461      89.37
 H      -2.570441    -1.555583    -1.577559      23.83
 C      -2.873036    -2.849570     0.178221     110.33
 O      -3.429525    -3.884213    -0.864276     251.73
 H      -3.464133    -3.467378    -1.717919      30.63
 H      -3.453698    -2.709811     1.080711      26.19
 H      -1.883867    -3.125732     0.474278      28.09
 C       1.668141    -1.124327    -1.335951      41.36
 H       2.205602    -1.487459    -2.194013      23.07
 C       1.513800     0.592998     0.548101      73.44
 H       1.977972     1.364781     1.161341      22.71
 C       0.077258     0.213853     0.812583       8.65
 O      -0.728210     0.953132     1.565574     195.36
 C      -0.260097     1.905684     2.555232      90.66
 H       0.616029     2.584033     2.022308      21.68
 H      -1.221923     2.271944     3.182977      21.08
 H       0.851789     1.455274     3.002531      22.71
 C      -0.520359    -0.703816    -0.083945      11.39
 O      -1.885652    -0.607726     0.109177     164.50
 C       0.304106    -1.367218    -1.099936      60.31
 H      -0.415415    -2.243258    -1.770201      18.37
 C       2.284116    -0.118088    -0.484178      23.03
 C       3.709818     0.086916    -0.688084     104.78
 H       4.018011    -0.368261    -1.642196      26.16
 O       4.157477     1.519967    -0.628927     185.44
 H       4.460779     1.817397     0.233087      27.07
 C       4.478991    -0.512517     0.513960      79.20
 H       4.354942    -0.333449     1.556197      26.84
 O       4.196716    -2.089941     0.521594     183.51
 H       4.841689    -2.692043     0.033609      29.55
 C       6.181731    -0.404058     0.513965      79.76
 O       6.528094     0.988552     0.876664     245.83
 H       6.729894     1.118890     1.807116      26.07
 H       6.478289    -0.812715    -0.436674      27.22
 H       6.756104    -1.300157     1.250214      25.60
55
name= lig-ACN-Water-frame_811
 C      -3.990598     0.724675    -2.959747      50.05
 H      -3.987822    -0.208289    -3.386736      23.12
 C      -3.797918     1.853191    -0.805929      41.36
 H      -3.638601     1.648782     0.322255      16.76
 C      -3.592908     3.122156    -1.439554      44.53
 O      -3.591746     4.490366    -0.900251     245.93
 C      -3.002731     4.608801     0.394935     129.72
 H      -3.024346     5.731146     0.927371      24.57
 H      -1.939992     4.115191     0.632234      24.92
 H      -3.558351     4.258212     1.348278      27.09
 C      -3.655171     3.167668    -2.876205       6.86
 O      -3.697662     4.246758    -3.749776     191.64
 H      -3.574871     5.070772    -3.374140      29.33
 C      -3.742369     1.879547    -3.593032      58.25
 H      -3.668000     1.966079    -4.675153      25.95
 C      -4.099711     0.650568    -1.564460      34.18
 C      -4.223541    -0.613709    -0.798554     103.26
 H      -4.966609    -1.328540    -1.411573      24.21
 O      -4.793478    -0.593169     0.543104     137.86
 H      -4.114402    -0.190464     1.163125      24.68
 C      -2.910715    -1.420540    -0.665392      66.28
 H      -2.343703    -1.741227    -1.574304      22.01
 C      -2.948687    -2.868604     0.052486     113.14
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 O      -3.388222    -3.844908    -0.748210     297.61
 H      -3.653647    -3.511645    -1.566629      33.77
 H      -3.618151    -2.965019     0.941874      24.40
 H      -1.976595    -3.089990     0.333611      27.38
 C       1.631581    -1.007212    -1.371206      41.65
 H       2.146130    -1.497774    -2.208748      22.99
 C       1.513582     0.515306     0.537765      73.97
 H       1.919043     1.389020     0.965513      22.84
 C       0.252083     0.246858     0.789167      -4.08
 O      -0.791511     0.970070     1.664963     132.77
 C      -0.168752     1.954200     2.596372      97.33
 H      -0.148442     2.971423     1.996884      21.35
 H      -1.041178     2.416166     3.305945      22.93
 H       0.394182     1.441282     3.608070      22.51
 C      -0.504342    -0.701764    -0.066441       1.17
 O      -1.887959    -0.615226     0.208233     133.23
 C       0.187786    -1.377110    -1.065510      62.82
 H      -0.317510    -2.309813    -1.855907      19.47
 C       2.296443    -0.222087    -0.478250      21.80
 C       3.843546     0.102053    -0.619695      88.84
 H       4.260333    -0.292112    -1.589111      26.11
 O       4.141509     1.472401    -0.613240     223.65
 H       4.561198     1.598179     0.299185      24.32
 C       4.561496    -0.688567     0.566524     109.99
 H       3.944809    -0.165900     1.230067      27.78
 O       4.198024    -2.004539     0.570292     249.98
 H       4.848722    -2.302700    -0.110412      30.49
 C       6.058183    -0.364067     0.588741      94.14
 O       6.616040     1.081994     0.956363     211.82
 H       6.829616     1.165088     1.941161      23.56
 H       6.631480    -0.362858    -0.307094      25.92
 H       6.436881    -0.996769     1.571286      24.80
55
name= lig-ACN-Water-frame_812
 C      -3.976830     0.549720    -2.975393      99.08
 H      -4.272266    -0.181268    -3.603317      26.72
 C      -3.677465     1.880627    -0.818756      68.83
 H      -3.605725     1.886620     0.238649      20.85
 C      -3.663431     3.201661    -1.442235       7.46
 O      -3.605033     4.455012    -0.899393     257.38
 C      -3.159723     4.632634     0.437613      95.71
 H      -3.115215     5.855881     0.487739      20.48
 H      -1.975556     4.265493     0.375353      23.14
 H      -3.918414     3.979914     0.956676      21.99
 C      -3.568035     3.116292    -2.853749      15.34
 O      -3.683445     4.336528    -3.725323     196.13
 H      -3.658770     5.073557    -3.042098      25.11
 C      -3.739174     1.908672    -3.553480      41.65
 H      -3.698662     2.025319    -4.573867      21.55
 C      -4.094402     0.683987    -1.503639       5.98
 C      -4.151621    -0.646487    -0.745668      84.11
 H      -4.890290    -1.392497    -1.389380      22.30
 O      -4.745938    -0.586722     0.520983     216.94
 H      -4.151088    -0.297170     1.320242      22.23
 C      -2.756773    -1.365175    -0.691919      73.67
 H      -2.464002    -1.318257    -1.835599      20.12
 C      -2.976357    -2.721265     0.035756      91.31
 O      -3.468007    -3.964847    -0.763629     251.62
 H      -3.265124    -3.765433    -1.819064      24.76
 H      -3.554735    -2.481675     0.997831      23.68
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 H      -2.038143    -2.927415     0.345654      27.52
 C       1.439247    -1.023701    -1.328570      55.12
 H       1.930211    -1.526781    -2.192147      22.76
 C       1.668596     0.488067     0.537815      51.10
 H       2.255696     1.146484     1.122287      18.98
 C       0.105862     0.314951     0.773634      -0.16
 O      -0.659879     0.943290     1.745788     180.49
 C      -0.264147     2.043384     2.652838      86.97
 H       0.433974     2.907852     2.281897      20.70
 H      -1.268367     2.116258     3.162737      20.52
 H       0.806966     1.565584     3.141427      20.32
 C      -0.543147    -0.637830    -0.016463      10.58
 O      -1.934892    -0.699608     0.223366     193.36
 C       0.177475    -1.333064    -1.086842      60.51
 H      -0.487060    -2.068897    -1.926923      17.52
 C       2.298668    -0.165009    -0.489011      19.73
 C       3.890437    -0.005389    -0.598959      79.10
 H       4.211950    -0.408327    -1.618515      22.49
 O       4.149077     1.497501    -0.565232     219.92
 H       4.775902     1.890139     0.120355      19.94
 C       4.548638    -0.524381     0.617651      95.64
 H       4.217803    -0.375568     1.591036      25.05
 O       4.281729    -2.034512     0.589777     245.79
 H       4.375952    -2.542824    -0.216960      29.85
 C       6.105244    -0.213068     0.772551     102.23
 O       6.585328     1.066129     0.937289     299.54
 H       6.781253     1.424900     1.935856      21.69
 H       6.348219    -0.647014    -0.187997      28.30
 H       6.621482    -1.099328     1.401647      27.02
55
name= lig-ACN-Water-frame_813
 C      -4.011271     0.702296    -2.878354      25.69
 H      -4.263258    -0.182547    -3.369438      19.11
 C      -3.664454     1.966196    -0.768097      47.54
 H      -3.734931     1.997807     0.239250      25.19
 C      -3.666197     3.144160    -1.541736      12.32
 O      -3.654140     4.422861    -1.016335     211.15
 C      -3.288317     4.617681     0.511644      85.91
 H      -3.442673     5.829948     0.684516      23.22
 H      -2.084047     4.368097     0.814247      20.86
 H      -3.769805     4.287109     1.415368      23.90
 C      -3.625520     3.140529    -2.980663      17.14
 O      -3.639168     4.334052    -3.581735     207.48
 H      -3.487467     5.220739    -2.950025      22.20
 C      -3.732170     1.876091    -3.605740      77.52
 H      -3.823703     1.800601    -4.607515      28.24
 C      -3.919942     0.671585    -1.524845      53.38
 C      -4.072848    -0.662512    -0.755429      91.78
 H      -4.756882    -1.459644    -1.440429      21.61
 O      -4.707486    -0.521909     0.590494     203.97
 H      -3.980768    -0.225243     1.197273      21.42
 C      -2.762925    -1.406263    -0.732721      58.57
 H      -2.125300    -1.359204    -1.760541      16.34
 C      -2.897490    -2.768624    -0.051393      95.34
 O      -3.567602    -3.976564    -0.753888     232.23
 H      -3.004073    -3.985408    -1.705616      25.09
 H      -3.843443    -2.586975     0.646795      20.21
 H      -2.104226    -3.119507     0.438845      26.91
 C       1.529879    -1.042828    -1.314828      42.43
 H       1.893493    -1.471370    -2.280743      19.81
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 C       1.548192     0.510038     0.637605      67.08
 H       2.079817     0.927510     1.476033      18.88
 C       0.262327     0.416358     0.753258      10.27
 O      -0.543771     0.932077     1.793227     203.41
 C      -0.203194     2.012700     2.664273      98.29
 H      -0.176093     2.890322     1.921277      20.21
 H      -0.955439     2.445137     3.350545      22.43
 H       0.593160     1.685229     3.606823      20.67
 C      -0.617346    -0.554152    -0.027368       6.22
 O      -1.904870    -0.711747     0.250160     192.96
 C       0.017358    -1.202937    -1.041179      66.44
 H      -0.599609    -1.962963    -1.800663      16.01
 C       2.270531    -0.163115    -0.545815      29.95
 C       3.763963     0.101803    -0.544826      84.95
 H       4.371158    -0.467251    -1.328831      23.25
 O       4.134836     1.531600    -0.591940     223.48
 H       4.911803     1.452848    -0.024997      21.19
 C       4.556544    -0.519215     0.784030      74.86
 H       3.944979    -0.126150     1.518137      24.17
 O       4.406168    -2.075820     0.644845     231.71
 H       4.259593    -1.995665    -0.344634      27.46
 C       6.181866    -0.319151     0.776175     100.08
 O       6.536605     1.128875     0.880817     222.36
 H       6.733722     1.273956     1.949313      22.63
 H       6.779556    -0.583840    -0.115180      26.09
 H       6.487307    -0.752354     1.754814      25.65
55
name= lig-ACN-Water-frame_814
 C      -4.010178     0.824252    -2.846567      53.85
 H      -4.063183    -0.194722    -3.318872      20.04
 C      -3.741061     1.951106    -0.772212      53.04
 H      -3.686921     2.017037     0.287137      14.46
 C      -3.620236     3.060415    -1.556137      14.91
 O      -3.670816     4.422096    -0.939397     251.02
 C      -3.421334     4.672856     0.472943      89.26
 H      -3.551357     5.841055     0.553355      22.70
 H      -2.215594     4.308017     0.680113      23.37
 H      -4.228569     4.044151     0.783574      28.12
 C      -3.716368     3.120142    -2.982771       2.76
 O      -3.586961     4.386838    -3.554122     168.65
 H      -3.342067     5.029872    -2.706405      18.56
 C      -3.798953     1.903779    -3.754836      58.78
 H      -3.806117     1.862674    -4.822702      26.12
 C      -3.753717     0.718824    -1.384114      51.55
 C      -4.036380    -0.598636    -0.766884      84.02
 H      -5.027672    -1.123997    -1.356747      23.36
 O      -4.618686    -0.445415     0.557891     192.28
 H      -4.039931    -0.378604     1.320713      23.38
 C      -2.739427    -1.497342    -0.696344      72.39
 H      -2.387037    -1.639397    -1.875293      19.03
 C      -2.958915    -2.989181    -0.073605     107.99
 O      -3.608178    -3.924643    -0.772387     327.92
 H      -3.317064    -4.147719    -1.615873      32.38
 H      -3.473394    -2.761102     1.029849      23.07
 H      -2.002029    -3.217858     0.217875      27.16
 C       1.459712    -0.988014    -1.306208      57.77
 H       2.019819    -1.490415    -2.108499      22.16
 C       1.642149     0.487344     0.616791      67.42
 H       2.197037     1.180605     1.304459      19.61
 C       0.099868     0.403939     0.819003      13.38
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 O      -0.526791     0.878101     1.894332     201.37
 C      -0.133848     2.063775     2.660356     105.03
 H       0.253569     3.016319     2.078138      21.99
 H      -1.079710     2.082203     3.114602      21.66
 H       0.957779     1.982767     3.235241      21.27
 C      -0.536791    -0.390785    -0.072697      12.13
 O      -1.905007    -0.656803     0.317452     167.32
 C       0.153127    -1.111023    -1.109924      63.57
 H      -0.403485    -1.949985    -1.656703      18.64
 C       2.217223    -0.092614    -0.394788      32.06
 C       3.786678     0.138365    -0.460095      78.47
 H       4.001871    -0.300884    -1.493200      24.02
 O       4.104511     1.538856    -0.618983     231.26
 H       4.914607     1.858562    -0.187306      22.55
 C       4.582330    -0.624491     0.787003     101.72
 H       4.381956    -0.402652     1.802131      25.25
 O       4.517335    -1.988240     0.684573     277.83
 H       4.258177    -2.348334    -0.194704      28.93
 C       6.131315    -0.337919     0.830386      91.30
 O       6.499310     1.166618     0.828471     241.08
 H       6.579754     1.487845     1.804602      24.22
 H       6.573682    -0.973474     0.036853      28.52
 H       6.489373    -0.810166     1.731036      28.70
55
name= lig-ACN-Water-frame_815
 C      -3.855210     0.738979    -2.891471      67.42
 H      -4.114042    -0.246794    -3.499709      23.61
 C      -3.721661     1.963652    -0.678392      56.37
 H      -3.709405     1.966551     0.493038      17.32
 C      -3.649230     3.198669    -1.472034      10.95
 O      -3.646961     4.409459    -1.018317     231.31
 C      -3.604321     4.624927     0.371627     120.00
 H      -3.630464     5.771325     0.551124      23.49
 H      -2.563035     4.233174     0.988944      24.52
 H      -4.254809     4.273798     1.122178      28.44
 C      -3.719938     3.171102    -2.971905      18.38
 O      -3.545601     4.421379    -3.555551     185.68
 H      -3.524348     5.134417    -2.893185      23.49
 C      -3.925311     1.993984    -3.661790      67.76
 H      -3.926617     1.922171    -4.805949      22.21
 C      -3.779602     0.791398    -1.523715      28.94
 C      -3.989554    -0.599030    -0.699588      84.14
 H      -4.731400    -1.201028    -1.540563      21.77
 O      -4.594277    -0.381039     0.542298     175.90
 H      -3.859504    -0.442212     1.201491      23.32
 C      -2.820899    -1.566288    -0.556513      73.85
 H      -2.140105    -1.546183    -1.570760      19.08
 C      -2.829198    -2.965119     0.038961      96.07
 O      -3.765563    -3.989430    -0.838818     185.71
 H      -3.497301    -3.584535    -1.628338      31.63
 H      -3.285779    -3.134093     1.183174      23.07
 H      -1.955439    -3.435776    -0.081951      25.79
 C       1.632077    -0.818497    -1.256530      49.26
 H       2.063630    -1.416974    -2.048897      24.85
 C       1.496136     0.624122     0.752591      72.39
 H       2.139554     1.371058     1.286832      18.89
 C       0.222208     0.421726     0.871471       5.54
 O      -0.563199     0.844565     2.030231     204.62
 C      -0.050314     2.118723     2.643950      98.49
 H      -0.065783     2.916121     1.812221      23.31
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 H      -0.522361     2.585136     3.425169      25.73
 H       0.878825     1.652167     3.257704      21.58
 C      -0.597575    -0.398585    -0.129498       0.72
 O      -1.873880    -0.687659     0.229728     155.28
 C       0.148888    -1.059593    -1.134898      65.03
 H      -0.308055    -1.725118    -1.819086      22.59
 C       2.325381    -0.110303    -0.346909      27.44
 C       3.814049     0.064680    -0.415222      88.11
 H       4.334238    -0.524490    -1.250698      24.25
 O       4.052505     1.595055    -0.636365     165.55
 H       4.822969     1.633725     0.032711      20.41
 C       4.632924    -0.530616     0.731969     103.86
 H       3.938953    -0.249451     1.493782      26.09
 O       4.573377    -2.066861     0.717491     251.77
 H       4.440260    -2.401056    -0.173427      31.49
 C       6.105031    -0.248088     0.878552     119.32
 O       6.452534     1.077185     0.758638     308.45
 H       6.505808     1.418554     1.601277      32.12
 H       6.647024    -0.572148    -0.051491      26.83
 H       6.456342    -0.675714     1.724468      29.89
55
name= lig-ACN-Water-frame_816
 C      -3.772854     0.763761    -2.982369      44.87
 H      -3.912858    -0.317469    -3.545056      21.68
 C      -3.667133     1.983817    -0.816361      57.70
 H      -3.750916     1.939345     0.415262      16.97
 C      -3.730941     3.139889    -1.492375      23.37
 O      -3.636384     4.518301    -1.051012     227.24
 C      -3.727812     4.674988     0.467859      98.44
 H      -3.668477     5.768443     0.528935      23.36
 H      -2.673535     4.121027     0.798496      22.61
 H      -4.689661     4.244651     0.623111      26.79
 C      -3.697158     3.251368    -2.832401      17.99
 O      -3.547277     4.428972    -3.606897     193.87
 H      -3.592024     5.177315    -3.062820      25.84
 C      -3.955139     2.008669    -3.526108      49.32
 H      -4.220169     2.193072    -4.685120      21.48
 C      -3.815962     0.732774    -1.512396      19.95
 C      -3.993696    -0.629302    -0.774474      77.53
 H      -4.886529    -1.414062    -1.159251      22.16
 O      -4.635230    -0.336392     0.578721     144.96
 H      -4.020149    -0.145872     1.405284      20.77
 C      -2.718448    -1.498905    -0.519923      99.50
 H      -2.531673    -1.860639    -1.623744      20.13
 C      -2.816949    -3.084409     0.021576      79.25
 O      -3.839672    -3.893488    -0.810629     200.89
 H      -3.997669    -3.663091    -1.807234      29.11
 H      -3.185472    -3.077434     1.204921      23.13
 H      -1.791513    -3.351209    -0.010810      25.26
 C       1.628901    -0.778397    -1.232933      40.42
 H       2.265919    -1.029049    -2.061871      22.22
 C       1.634171     0.722850     0.732079      65.17
 H       1.932851     1.218340     1.654457      16.18
 C       0.092258     0.368469     0.923893     -24.53
 O      -0.622752     0.872635     2.131305     176.55
 C       0.050908     2.075476     2.635583     103.44
 H       0.179619     2.806736     1.652887      22.89
 H      -0.751485     2.409831     3.232677      24.27
 H       1.116655     2.194839     2.910237      23.93
 C      -0.497187    -0.463974    -0.053073      16.33
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 O      -1.848278    -0.729762     0.213730     211.90
 C       0.241092    -0.950427    -1.175310      64.31
 H      -0.227499    -1.402805    -1.909550      23.10
 C       2.351281    -0.011578    -0.195508      11.40
 C       3.881078     0.075168    -0.504721      82.52
 H       4.077781    -0.298325    -1.567337      22.78
 O       4.048764     1.542598    -0.604542     193.72
 H       4.706954     2.009965    -0.037731      21.46
 C       4.538039    -0.530097     0.807747      96.27
 H       4.268818    -0.135343     1.790761      22.80
 O       4.589615    -2.107405     0.744218     222.56
 H       4.803801    -2.140043    -0.244019      28.61
 C       6.127905    -0.295317     0.816706      98.22
 O       6.448214     1.172311     0.736662     227.58
 H       6.481919     1.529294     1.683398      26.97
 H       6.556524    -0.965576     0.047340      30.29
 H       6.426867    -0.632752     1.706973      31.59
55
name= lig-ACN-Water-frame_817
 C      -3.832880     0.789094    -2.891757      95.65
 H      -3.767316    -0.059936    -3.763038      22.14
 C      -3.704986     1.880875    -0.898943      59.70
 H      -3.665509     1.908285     0.346979      12.93
 C      -3.710831     3.306468    -1.476281      52.28
 O      -3.618918     4.602489    -0.947102     308.57
 C      -3.836537     4.730989     0.435779     141.25
 H      -3.684037     5.657414     0.852811      25.72
 H      -3.242349     4.014333     1.171066      22.41
 H      -4.793283     4.338086     0.732072      30.41
 C      -3.741220     3.242827    -2.941155      26.55
 O      -3.607453     4.393624    -3.645446     155.19
 H      -3.432742     5.153852    -2.930665      24.07
 C      -3.890169     2.078556    -3.581315      45.83
 H      -4.082622     2.072327    -4.778627      20.08
 C      -3.766335     0.612686    -1.538828      39.49
 C      -4.053700    -0.650337    -0.629658      92.96
 H      -4.825413    -1.158595    -1.452209      18.76
 O      -4.707544    -0.296183     0.585106     228.46
 H      -3.904052    -0.348596     1.247655      21.98
 C      -2.685062    -1.580589    -0.668635      55.92
 H      -2.097700    -1.381025    -1.589594      20.18
 C      -2.905595    -3.032792    -0.094668     103.49
 O      -3.858721    -3.755918    -0.698809     244.60
 H      -3.298067    -3.679586    -1.667558      24.77
 H      -3.291184    -3.005139     1.043122      22.10
 H      -2.042717    -3.689949    -0.144274      23.23
 C       1.686398    -0.685424    -1.173080      51.99
 H       2.086142    -1.032364    -2.111216      19.68
 C       1.538368     0.648063     0.836479      59.67
 H       2.297091     1.149649     1.384592      19.07
 C       0.191507     0.385677     1.022578      12.19
 O      -0.535196     0.844579     2.063994     222.22
 C       0.042154     2.105059     2.552340     108.47
 H      -0.047666     3.022322     1.788280      20.67
 H      -0.553549     2.449051     3.386881      23.97
 H       0.805973     1.690709     3.146471      22.97
 C      -0.418173    -0.521611     0.049862      -5.38
 O      -1.773966    -0.749745     0.278297     179.57
 C       0.262942    -0.864819    -1.168752      68.50
 H      -0.139179    -1.255771    -1.918033      21.57
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 C       2.302292     0.037097    -0.244618      35.97
 C       3.784373     0.190044    -0.385078      84.35
 H       4.148971    -0.465742    -1.247615      24.37
 O       4.095658     1.554197    -0.601766     223.70
 H       4.839612     1.577293     0.021959      20.59
 C       4.688630    -0.631645     0.777934      92.29
 H       4.015876    -0.505028     1.682218      23.26
 O       4.529452    -2.008037     0.739251     277.66
 H       5.089132    -2.511067     0.085578      29.84
 C       6.106449    -0.311588     0.824914     113.43
 O       6.464356     1.255081     0.726001     171.08
 H       6.534737     1.460374     1.796287      22.97
 H       6.680990    -0.625669    -0.061498      28.00
 H       6.579333    -0.660827     1.637145      30.88
55
name= lig-ACN-Water-frame_818
 C      -3.914506     0.771259    -2.990032      29.49
 H      -4.044628    -0.298729    -3.492511      18.06
 C      -3.740757     2.022800    -0.828385      50.22
 H      -3.696168     1.916035     0.363528      11.52
 C      -3.661871     3.204460    -1.534920      20.50
 O      -3.579259     4.593941    -0.894956     235.16
 C      -3.971078     4.729992     0.575723     108.03
 H      -3.705472     5.663202     0.649991      28.24
 H      -3.240156     4.059277     1.050395      28.49
 H      -5.043042     4.696548     0.729978      29.29
 C      -3.773749     3.285224    -2.919145       6.07
 O      -3.684790     4.454503    -3.701711     186.39
 H      -3.388789     5.342515    -3.154387      21.62
 C      -3.806989     1.965933    -3.670154      59.46
 H      -3.577578     1.926875    -4.821692      24.83
 C      -3.754100     0.751562    -1.505155      56.77
 C      -4.014669    -0.653949    -0.723172      82.12
 H      -4.849125    -1.456129    -1.113410      23.93
 O      -4.680870    -0.317339     0.593371     205.38
 H      -4.202166    -0.375346     1.424402      24.43
 C      -2.688860    -1.482033    -0.672360      93.77
 H      -2.441764    -1.610389    -1.668055      23.03
 C      -2.821561    -2.851553    -0.051324      89.07
 O      -3.949618    -3.683473    -0.762988     186.61
 H      -3.793940    -4.086413    -1.671433      29.02
 H      -3.100531    -2.598510     1.041672      24.39
 H      -1.793623    -3.279985    -0.003936      25.30
 C       1.624752    -0.655386    -1.298478      57.22
 H       2.331059    -1.087048    -2.010985      23.64
 C       1.702430     0.564705     0.911291      65.39
 H       1.872691     1.375895     1.532177      17.47
 C       0.271510     0.275090     1.030598     -17.25
 O      -0.510056     0.878120     1.983564     195.88
 C      -0.026467     2.082457     2.630207     111.91
 H       0.279247     2.797041     1.775482      23.33
 H      -0.827115     2.467653     3.343737      23.28
 H       0.914671     2.073045     3.038555      25.32
 C      -0.454210    -0.505436     0.083881      10.03
 O      -1.740268    -0.826107     0.368121     145.28
 C       0.239880    -0.866780    -1.078575      66.62
 H      -0.292716    -1.376019    -1.702487      23.15
 C       2.297365     0.078613    -0.225833       8.51
 C       3.790075     0.132744    -0.281701      92.98
 H       3.966316    -0.322459    -1.313032      24.03
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 O       4.214827     1.620603    -0.549071     186.77
 H       5.052479     1.920730    -0.163338      19.08
 C       4.623977    -0.560128     0.782009      87.24
 H       4.472404    -0.131226     1.866176      23.12
 O       4.445144    -2.051331     0.693794     275.50
 H       5.279066    -2.366706     0.347669      30.99
 C       6.282207    -0.135875     0.794256     104.37
 O       6.437578     1.212695     0.809305     284.88
 H       6.460178     1.658192     1.715460      25.35
 H       6.601531    -0.511463    -0.210402      28.62
 H       6.685251    -0.673539     1.568659      30.45
55
name= lig-ACN-Water-frame_819
 C      -3.921732     0.746383    -2.915146      72.06
 H      -4.151930    -0.204328    -3.439756      20.84
 C      -3.723556     2.054653    -0.761574      51.49
 H      -3.838164     2.214534     0.327425      19.53
 C      -3.670786     3.279597    -1.503975      23.89
 O      -3.571931     4.451123    -0.889665     207.43
 C      -3.984244     4.747558     0.563689     120.89
 H      -3.776408     5.646506     0.790340      27.52
 H      -3.665143     4.189518     1.305119      31.89
 H      -5.016402     4.389756     0.426932      27.09
 C      -3.723043     3.190860    -3.025852      14.78
 O      -3.762741     4.492310    -3.747127     187.76
 H      -3.636664     5.094067    -3.030950      27.87
 C      -3.707710     1.994435    -3.687587      60.51
 H      -3.662210     2.088608    -4.789285      24.39
 C      -3.921158     0.845283    -1.531233      29.24
 C      -3.965853    -0.481464    -0.744955      92.47
 H      -4.612811    -1.111231    -1.532032      21.76
 O      -4.625139    -0.380663     0.587721     199.09
 H      -3.859046    -0.159811     1.102269      24.70
 C      -2.697969    -1.314503    -0.590800      92.79
 H      -2.179924    -1.257506    -1.443577      23.88
 C      -2.863186    -2.768632    -0.046661      96.87
 O      -3.960749    -3.595546    -0.725532     204.92
 H      -3.597221    -3.523908    -1.547761      31.97
 H      -3.258524    -2.906539     0.920705      23.90
 H      -1.844771    -3.321189    -0.168648      23.47
 C       1.589037    -0.580996    -1.233905      35.40
 H       1.941185    -1.015746    -2.192476      26.30
 C       1.683528     0.539277     0.938270      60.10
 H       2.408831     0.954172     1.585341      19.44
 C       0.306742     0.265661     1.084621       6.52
 O      -0.532288     0.894969     1.979098     190.01
 C      -0.028347     2.094191     2.640374     107.06
 H      -0.083587     2.988961     2.005838      24.71
 H      -1.058577     2.248780     3.179640      24.07
 H       0.511491     1.809359     3.413512      27.22
 C      -0.430962    -0.498562     0.045132     -10.09
 O      -1.775175    -0.889291     0.404978     177.77
 C       0.213738    -1.005275    -1.074563      62.62
 H      -0.205891    -1.629020    -1.820326      21.70
 C       2.397376     0.042033    -0.235111     -11.70
 C       3.952897     0.209293    -0.390856      85.01
 H       4.413497    -0.400898    -1.257021      23.01
 O       4.247352     1.638504    -0.501731     180.61
 H       5.144202     1.653085    -0.005487      17.12
 C       4.698616    -0.455857     0.874175      72.96
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 H       4.145378    -0.270777     1.939091      20.96
 O       4.387272    -2.023011     0.675769     223.49
 H       5.313779    -2.375550     0.478778      29.03
 C       6.266798    -0.168661     0.674876     107.96
 O       6.466621     1.312266     0.920419     278.19
 H       6.467499     1.361969     1.837198      29.21
 H       6.786838    -0.431796    -0.263885      27.04
 H       6.858017    -0.653263     1.449075      28.68
55
name= lig-ACN-Water-frame_820
 C      -3.887184     0.878824    -2.887704      63.01
 H      -3.944033    -0.019186    -3.381644      22.66
 C      -3.768251     2.070247    -0.831593      56.46
 H      -3.709002     1.993485     0.168762      23.37
 C      -3.701818     3.238448    -1.563674      24.46
 O      -3.506004     4.467980    -0.879106     256.02
 C      -4.053635     4.674831     0.421673     136.72
 H      -3.952715     5.629386     0.472548      25.68
 H      -3.438830     4.220940     1.002023      32.49
 H      -5.140188     4.621503     0.665586      27.43
 C      -3.634890     3.285310    -2.985595      21.56
 O      -3.816817     4.399086    -3.702451     219.65
 H      -3.855736     5.149855    -3.143882      30.19
 C      -3.685802     1.985663    -3.668871      70.70
 H      -3.852216     1.831262    -4.668615      25.30
 C      -4.006864     0.911405    -1.458625      44.83
 C      -4.018588    -0.364781    -0.723829     105.17
 H      -4.682832    -1.161081    -1.291162      24.09
 O      -4.556743    -0.434215     0.536492     203.42
 H      -4.102831     0.012210     1.350135      21.41
 C      -2.643790    -1.247863    -0.574858      73.02
 H      -2.248727    -1.305017    -1.482299      26.08
 C      -2.994382    -2.761878    -0.058004     115.31
 O      -3.903410    -3.488686    -0.734827     261.72
 H      -4.052361    -3.298069    -1.678549      27.87
 H      -3.050945    -2.622081     0.920945      27.64
 H      -1.951749    -3.295881    -0.242991      25.24
 C       1.626624    -0.628064    -1.219584      56.15
 H       2.168358    -0.678684    -2.188741      23.49
 C       1.743876     0.461727     0.884559      60.44
 H       2.067341     0.795758     1.872177      20.69
 C       0.301677     0.367857     1.018860     -21.85
 O      -0.541283     0.864972     1.971976     206.73
 C      -0.205772     2.095393     2.739837     114.56
 H       0.441154     2.658730     2.209757      28.10
 H      -1.039327     2.557243     3.434581      23.51
 H       0.560441     1.816547     3.297851      27.76
 C      -0.459694    -0.554595     0.085133     -15.08
 O      -1.712933    -0.806429     0.506945     175.46
 C       0.276130    -1.068895    -1.037515      68.15
 H      -0.144931    -1.739105    -1.867775      21.86
 C       2.438387    -0.010856    -0.289639      28.34
 C       3.997895     0.247670    -0.413264      81.67
 H       4.399661    -0.258565    -1.381794      26.19
 O       4.281133     1.639881    -0.462209     197.81
 H       4.980427     1.958129     0.157734      21.41
 C       4.768729    -0.545406     0.769686      89.49
 H       4.406350    -0.017794     1.834521      23.36
 O       4.400990    -1.858076     0.688506     290.54
 H       5.078666    -2.569989     0.640815      29.72
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 C       6.220949    -0.177447     0.720136      91.67
 O       6.506056     1.344361     0.976179     216.65
 H       6.944862     1.561365     1.788346      25.30
 H       6.353261    -0.256997    -0.396002      28.11
 H       6.842086    -0.901322     1.275432      28.94
55
name= lig-ACN-Water-frame_821
 C      -3.870082     0.860804    -2.883833      37.42
 H      -3.886794    -0.007461    -3.332213      24.68
 C      -3.838455     2.156760    -0.777222      37.65
 H      -3.691492     2.273779     0.175380      15.23
 C      -3.652974     3.295153    -1.536692      27.42
 O      -3.476450     4.529554    -1.004418     244.32
 C      -4.047993     4.695711     0.365145     117.89
 H      -4.065067     5.638507     0.467745      26.77
 H      -3.565715     4.282139     1.094810      34.82
 H      -5.003179     4.060422     0.271947      31.64
 C      -3.640474     3.247207    -2.954139      30.52
 O      -3.842687     4.393320    -3.714543     220.89
 H      -3.788778     5.296792    -3.114292      26.28
 C      -3.717655     2.081060    -3.635674      37.18
 H      -3.534791     2.143644    -4.618049      18.64
 C      -3.957800     0.848604    -1.488051      42.40
 C      -3.956604    -0.521851    -0.690446     107.71
 H      -4.659685    -1.145041    -1.339342      24.53
 O      -4.663029    -0.429597     0.635332     161.26
 H      -3.921734    -0.086211     1.303292      21.00
 C      -2.665543    -1.277350    -0.603716      83.98
 H      -2.117609    -1.258512    -1.464647      21.80
 C      -2.855761    -2.609697    -0.058327      99.45
 O      -4.036685    -3.450698    -0.780714     141.40
 H      -3.789165    -3.212509    -1.834414      24.89
 H      -3.317196    -2.670945     0.742035      26.19
 H      -1.819802    -3.194847     0.063749      23.82
 C       1.727451    -0.727853    -1.302729      33.02
 H       2.108460    -1.156465    -2.262520      20.56
 C       1.717654     0.439477     0.903282      60.25
 H       2.359938     1.104209     1.532090      18.08
 C       0.302500     0.404933     0.876891      -0.55
 O      -0.591173     0.876297     2.000346     167.90
 C      -0.156145     2.010588     2.830100     119.14
 H       0.097218     2.720101     2.198038      25.60
 H      -1.203478     2.520701     2.995442      21.20
 H       0.226983     1.814337     3.708357      26.75
 C      -0.332786    -0.564429     0.124317       0.78
 O      -1.719525    -0.707994     0.505609     141.97
 C       0.384097    -1.046376    -0.984433      61.71
 H      -0.351052    -1.719421    -1.682790      17.13
 C       2.449020     0.015193    -0.208671      12.38
 C       3.929070     0.198892    -0.401675      92.22
 H       4.132333    -0.074537    -1.462598      23.37
 O       4.304953     1.710292    -0.418696     173.84
 H       4.691380     1.799098     0.441130      25.09
 C       4.746987    -0.391850     0.710445      72.55
 H       4.292669     0.010372     1.799884      20.88
 O       4.389346    -1.841175     0.711255     274.28
 H       5.257560    -2.216460     0.849005      29.55
 C       6.303988    -0.084920     0.627383     101.44
 O       6.542868     1.240250     0.962364     340.23
 H       6.656001     1.215482     1.928375      27.82
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 H       6.836668    -0.260081    -0.361726      25.62
 H       6.899679    -0.757272     1.382762      26.36
55
name= lig-ACN-Water-frame_822
 C      -3.837756     0.778545    -2.907560      27.65
 H      -3.880121    -0.032707    -3.482847      20.17
 C      -3.853488     2.096549    -0.723823      54.03
 H      -4.033235     2.043757     0.288851      16.52
 C      -3.587730     3.342979    -1.521163       6.69
 O      -3.435876     4.666601    -1.061871     269.02
 C      -4.043413     4.707002     0.297616     105.74
 H      -4.377873     5.605311     0.520359      27.10
 H      -3.417703     4.364398     0.961400      32.95
 H      -5.057668     4.201636     0.305526      29.74
 C      -3.747615     3.306477    -2.950434       4.20
 O      -3.814870     4.468921    -3.745658     198.81
 H      -3.501476     5.210192    -3.071146      21.85
 C      -3.714596     2.034574    -3.634200      51.83
 H      -3.627168     2.019608    -4.678495      26.58
 C      -3.842606     0.831065    -1.407209      35.48
 C      -4.028709    -0.523209    -0.675087      90.65
 H      -4.552866    -1.266808    -1.276698      23.98
 O      -4.730447    -0.406061     0.677567     205.40
 H      -4.133237    -0.449940     1.441678      23.33
 C      -2.576691    -1.235982    -0.574741      75.20
 H      -2.275830    -1.151579    -1.615079      21.03
 C      -2.935724    -2.734688    -0.037317     103.11
 O      -3.961296    -3.335717    -0.834347     212.08
 H      -3.604385    -3.642729    -1.770985      25.62
 H      -3.095696    -2.459517     0.864888      27.13
 H      -1.975025    -3.501373    -0.102291      22.88
 C       1.781435    -0.815769    -1.191745      30.24
 H       2.395480    -1.310468    -1.957439      20.21
 C       1.709269     0.601227     0.863320      86.33
 H       2.203335     1.346606     1.553454      18.49
 C       0.304258     0.430952     1.092665      14.10
 O      -0.519656     0.854921     1.964256     223.26
 C      -0.218600     2.003486     2.826265     121.54
 H       0.466328     2.564002     2.514514      29.02
 H      -1.182606     2.393533     3.224235      21.95
 H       0.282898     1.535315     3.577486      26.21
 C      -0.337134    -0.501444     0.097554       2.36
 O      -1.693925    -0.636333     0.345248     181.61
 C       0.391197    -1.072548    -0.997175      80.50
 H       0.030734    -1.883867    -1.901536      16.14
 C       2.382983    -0.056813    -0.307788      35.16
 C       3.872146     0.344562    -0.438707     107.27
 H       4.343151    -0.223607    -1.246354      21.26
 O       4.253321     1.728013    -0.366465     214.90
 H       4.593931     2.033120     0.531415      21.22
 C       4.752045    -0.326908     0.659625      50.03
 H       4.470555     0.249469     1.746554      19.19
 O       4.447673    -1.838836     0.746064     233.42
 H       5.248955    -2.350313     1.077916      27.73
 C       6.358215    -0.140904     0.506573      85.06
 O       6.620240     1.229261     0.964045     314.83
 H       6.658786     1.340328     1.986927      27.32
 H       6.859237    -0.419523    -0.477310      26.67
 H       6.609207    -0.859431     1.362193      26.71
55
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name= lig-ACN-Water-frame_823
 C      -3.751538     0.821044    -2.823625      59.07
 H      -3.806144    -0.159804    -3.217521      22.98
 C      -3.779609     2.061950    -0.792212      50.10
 H      -4.016047     2.119970     0.304743      18.04
 C      -3.611069     3.318821    -1.575317       3.52
 O      -3.453210     4.712451    -1.032942     235.97
 C      -4.051365     4.805929     0.279788     110.27
 H      -4.071275     5.797510     0.306084      25.18
 H      -3.329983     4.488936     0.915458      30.78
 H      -4.875599     4.077732     0.410177      28.51
 C      -3.780526     3.286511    -2.974295       7.98
 O      -3.741919     4.518380    -3.721439     199.79
 H      -3.501066     5.234007    -3.224725      28.09
 C      -3.753588     1.956303    -3.593107      69.23
 H      -3.991447     1.815626    -4.671442      24.53
 C      -3.833240     0.836044    -1.445235      29.27
 C      -4.022231    -0.456047    -0.585682     101.83
 H      -4.718920    -0.966925    -1.158455      23.49
 O      -4.749972    -0.383718     0.635107     238.01
 H      -4.128359    -0.303595     1.365114      25.42
 C      -2.630081    -1.301587    -0.593826      75.12
 H      -2.176926    -1.453916    -1.623106      18.79
 C      -2.877868    -2.767812    -0.061418     105.05
 O      -3.918659    -3.287720    -0.889922     255.61
 H      -3.503755    -3.420473    -1.689800      31.84
 H      -3.359493    -3.055398     0.843282      23.35
 H      -1.835232    -3.441043    -0.138079      22.28
 C       1.754730    -0.959065    -1.067584      32.90
 H       2.325685    -1.388668    -1.891219      23.22
 C       1.694070     0.763255     0.766377      81.62
 H       2.255595     1.385009     1.491127      21.51
 C       0.413326     0.245742     1.013031       1.69
 O      -0.569972     0.906751     1.999592     179.06
 C      -0.170353     1.929905     2.924231     126.19
 H       0.375544     2.517050     2.396996      29.85
 H      -0.942801     2.621295     3.123976      25.77
 H       0.266718     1.612957     3.849066      26.52
 C      -0.310524    -0.424293    -0.001572      13.58
 O      -1.662272    -0.540898     0.209929     192.51
 C       0.365599    -1.126858    -1.003857      53.39
 H      -0.489210    -1.849999    -1.685494      15.49
 C       2.429337     0.148345    -0.195217      20.61
 C       3.948358     0.329949    -0.413326     105.70
 H       4.059221     0.257556    -1.462729      25.14
 O       4.125140     1.795400    -0.382746     195.44
 H       4.574294     2.003138     0.477732      25.36
 C       4.834723    -0.435112     0.648794      85.72
 H       4.574949     0.085990     1.780652      22.06
 O       4.496438    -1.748769     0.762219     272.96
 H       5.248354    -2.190433     1.242455      29.17
 C       6.268199    -0.199776     0.546157      95.92
 O       6.742890     1.250419     0.919566     191.37
 H       7.275955     1.172782     1.797580      26.28
 H       6.489372    -0.156698    -0.529681      28.50
 H       7.065045    -0.995229     0.955175      28.03
55
name= lig-ACN-Water-frame_824
 C      -3.725821     0.768366    -2.768735      60.94
 H      -3.710671    -0.159534    -3.431931      23.22
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 C      -3.698390     2.214279    -0.832900      49.55
 H      -3.446994     2.357318     0.334358      17.90
 C      -3.676099     3.352731    -1.585194      20.18
 O      -3.514293     4.553735    -1.078426     246.65
 C      -3.944557     4.933650     0.346598     126.90
 H      -4.268625     5.906672     0.485788      25.29
 H      -3.421651     4.612150     1.180657      30.30
 H      -4.979885     4.571854     0.432298      29.10
 C      -3.690566     3.256513    -3.034889      24.36
 O      -3.683260     4.464935    -3.708465     197.74
 H      -3.598698     5.030448    -2.905545      23.84
 C      -3.865436     2.028014    -3.603529      59.42
 H      -3.839327     1.988054    -4.793922      21.83
 C      -3.814524     0.883439    -1.343526      29.06
 C      -3.988377    -0.476363    -0.665658     100.22
 H      -4.555338    -1.065921    -1.239113      24.63
 O      -4.692835    -0.321568     0.632799     224.66
 H      -4.118738     0.183174     1.338591      22.10
 C      -2.732197    -1.347574    -0.543827      75.09
 H      -2.495642    -1.411206    -1.692012      18.75
 C      -2.789715    -2.764493    -0.053528      87.73
 O      -3.910984    -3.344410    -1.024805     186.64
 H      -3.722548    -3.118774    -1.900630      30.65
 H      -3.062452    -2.725088     1.088420      22.54
 H      -1.676762    -3.254753    -0.221579      21.93
 C       1.801697    -0.903793    -0.940072      46.95
 H       2.342285    -1.474400    -1.692640      23.65
 C       1.667631     0.831037     0.790996      77.36
 H       2.041796     1.658789     1.378962      20.50
 C       0.324277     0.371930     0.994577      -1.58
 O      -0.593047     0.839355     1.977783     165.80
 C      -0.041016     1.940741     2.952582     122.96
 H       0.624821     2.511346     2.614846      31.40
 H      -0.977345     2.302563     3.113867      24.71
 H       0.323029     1.505661     3.900245      26.98
 C      -0.354045    -0.455269    -0.022206      10.48
 O      -1.716456    -0.431844     0.139931     151.36
 C       0.399874    -1.159379    -0.968319      70.36
 H      -0.013865    -1.980031    -1.945568      16.75
 C       2.453731     0.046890    -0.266692      36.75
 C       3.914350     0.337711    -0.424697      83.52
 H       4.361036    -0.246993    -1.196895      25.61
 O       4.043839     1.881407    -0.370485     169.53
 H       4.602210     2.143961     0.349242      25.73
 C       4.820464    -0.330391     0.779297      62.35
 H       4.303107     0.236798     1.744426      21.90
 O       4.512707    -1.808719     0.748142     282.30
 H       5.160480    -2.304086     1.252171      30.12
 C       6.426978    -0.064113     0.420815      76.05
 O       6.855765     1.168460     0.860762     274.78
 H       7.140425     1.162794     1.803843      28.71
 H       6.492194    -0.179399    -0.692482      27.88
 H       7.029002    -0.996545     0.991167      25.73
55
name= lig-ACN-Water-frame_825
 C      -3.847286     0.898341    -2.828140      55.23
 H      -3.845920    -0.247312    -3.183974      23.00
 C      -3.628349     2.177269    -0.744556      47.91
 H      -3.336558     2.401911     0.456854      16.05
 C      -3.712859     3.269583    -1.606463      10.84
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 O      -3.543275     4.617931    -1.015020     257.22
 C      -3.948831     5.006092     0.357935      94.70
 H      -3.565942     5.953951     0.093680      23.04
 H      -3.080814     4.606060     0.892542      27.73
 H      -4.879729     4.563061     0.675743      29.72
 C      -3.676536     3.257258    -3.004411      19.91
 O      -3.616216     4.427247    -3.700194     201.17
 H      -3.657172     5.373843    -3.189653      24.46
 C      -3.860050     1.956128    -3.613163      74.40
 H      -3.716229     1.826289    -4.814767      21.28
 C      -3.733496     0.924155    -1.412380      19.72
 C      -4.036821    -0.470789    -0.627732     100.29
 H      -4.724362    -0.960220    -1.131426      25.10
 O      -4.639859    -0.254591     0.619560     219.09
 H      -3.951622     0.170253     1.276295      22.73
 C      -2.664770    -1.216702    -0.614934      90.41
 H      -2.197435    -1.278735    -1.707382      19.15
 C      -2.848077    -2.747264    -0.198562      89.58
 O      -3.837659    -3.404225    -0.974696     240.04
 H      -3.370943    -3.409091    -1.909018      26.83
 H      -3.186025    -2.905422     1.020898      21.66
 H      -1.862493    -3.428451    -0.380761      20.70
 C       1.853905    -0.949950    -1.011417      39.52
 H       2.553489    -1.473782    -1.678916      22.12
 C       1.603509     0.735342     0.752061      71.03
 H       2.077066     1.553220     1.241682      20.19
 C       0.221166     0.538163     0.867138      16.41
 O      -0.496700     0.837726     2.010085     221.12
 C      -0.049342     1.862633     2.925845     126.89
 H       0.571399     2.387001     2.485865      30.12
 H      -0.640897     2.526755     3.384291      25.83
 H       0.530724     1.158673     3.602007      23.73
 C      -0.400377    -0.492818     0.049481      14.98
 O      -1.830974    -0.382372     0.101847     194.47
 C       0.458677    -1.153231    -0.888423      63.88
 H      -0.026416    -1.947974    -1.861428      16.87
 C       2.411574     0.093490    -0.138996      26.88
 C       3.924272     0.353038    -0.293859      99.43
 H       4.268895     0.179580    -1.289846      24.22
 O       4.009719     1.859527    -0.405285     186.34
 H       4.762070     2.080264     0.233988      23.37
 C       4.801308    -0.218959     0.804014      72.35
 H       4.930084     0.009972     1.954866      20.22
 O       4.523777    -1.801381     0.726107     224.45
 H       5.284303    -2.226778     1.226936      27.09
 C       6.411593    -0.063859     0.357129      69.28
 O       7.020948     1.200725     0.824731     252.78
 H       6.740544     1.264195     1.735640      30.23
 H       6.642892    -0.083391    -0.739890      24.31
 H       6.993913    -1.058070     0.903222      24.94
55
name= lig-ACN-Water-frame_826
 C      -3.984667     0.850368    -2.781251      53.72
 H      -4.312339    -0.140783    -3.442635      21.06
 C      -3.570418     2.084105    -0.739197      50.11
 H      -3.743676     1.963936     0.511876      16.14
 C      -3.659578     3.341290    -1.421283      13.16
 O      -3.616974     4.658672    -1.067411     257.85
 C      -3.740756     5.042754     0.305016     133.39
 H      -3.943348     6.113510     0.649857      23.72
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 H      -3.244264     4.506616     1.179892      26.79
 H      -4.772792     4.953930     0.627909      27.72
 C      -3.754088     3.242962    -2.966779       5.92
 O      -3.553074     4.425281    -3.781465     156.10
 H      -3.529401     5.084167    -3.000392      22.97
 C      -3.767826     2.061445    -3.687997      47.16
 H      -3.901763     1.914182    -4.877180      22.61
 C      -3.773131     0.884983    -1.409434      43.28
 C      -4.027018    -0.342961    -0.723401      96.53
 H      -4.695585    -0.894531    -1.241844      24.77
 O      -4.596279    -0.189851     0.670552     207.00
 H      -3.914055    -0.252895     1.361171      23.86
 C      -2.672478    -1.221839    -0.787507      59.60
 H      -2.306639    -1.159489    -1.928591      19.48
 C      -2.817046    -2.695592    -0.292716      81.27
 O      -3.812922    -3.482928    -0.936147     239.14
 H      -3.655568    -3.854439    -1.976671      25.21
 H      -3.262672    -2.668653     0.937297      20.90
 H      -1.702954    -3.126987    -0.227567      21.74
 C       1.863204    -0.916430    -0.985929      42.09
 H       2.295930    -1.429682    -1.870331      22.64
 C       1.541416     0.760095     0.768918      56.70
 H       1.982486     1.268797     1.610717      22.90
 C       0.183714     0.520862     0.817519       7.58
 O      -0.553081     0.896771     2.006647     187.29
 C       0.112243     1.780249     2.927549     130.20
 H       0.616468     2.489237     2.498846      29.09
 H      -0.815690     2.135785     3.207908      24.12
 H       0.697621     1.496824     3.842229      25.45
 C      -0.419065    -0.423405     0.017138      11.17
 O      -1.795799    -0.385672     0.155471     167.46
 C       0.415537    -1.160271    -0.843560      81.16
 H      -0.359873    -2.030891    -1.448198      14.93
 C       2.438232    -0.001064    -0.147678      21.27
 C       3.853835     0.445519    -0.172615     111.18
 H       4.092428    -0.214340    -1.013356      23.38
 O       4.039874     1.844002    -0.386749     271.64
 H       4.865560     2.265656    -0.034611      21.73
 C       4.979294    -0.338970     0.731005      90.55
 H       4.592801     0.191415     1.688084      22.35
 O       4.557336    -1.632927     0.715607     275.49
 H       5.294922    -2.238503     1.103336      26.60
 C       6.357498    -0.080839     0.355376      77.96
 O       7.123061     1.234818     0.796057     202.54
 H       7.046412     1.473141     1.789626      28.27
 H       6.399760    -0.082900    -0.783191      25.85
 H       7.114174    -1.001613     0.797294      24.43
55
name= lig-ACN-Water-frame_827
 C      -4.053219     0.893957    -2.936788      62.02
 H      -4.468214    -0.166955    -3.350321      21.26
 C      -3.602835     2.162118    -0.724933      55.55
 H      -3.606558     2.093810     0.520389      18.90
 C      -3.596890     3.330447    -1.516745      20.65
 O      -3.643024     4.727582    -1.108030     197.15
 C      -3.710220     5.091293     0.408478      69.06
 H      -3.190438     6.183098     0.246177      21.92
 H      -2.876863     4.323710     0.862685      22.57
 H      -4.678587     4.692904     0.553180      24.88
 C      -3.697075     3.297075    -2.898988      21.21
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 O      -3.530226     4.402650    -3.732273     200.54
 H      -3.317977     5.173007    -3.333843      28.32
 C      -3.829513     2.048834    -3.551018      63.42
 H      -3.845123     2.258068    -4.663989      21.35
 C      -3.916237     0.966855    -1.524756       5.78
 C      -4.017065    -0.444558    -0.711852      90.36
 H      -4.796786    -0.983619    -1.169780      22.82
 O      -4.537282    -0.167217     0.658431     240.56
 H      -3.859481    -0.167562     1.321084      23.50
 C      -2.753429    -1.186360    -0.849999      67.21
 H      -2.294704    -1.099065    -1.947400      20.31
 C      -2.750457    -2.597743    -0.306811      76.76
 O      -3.838938    -3.594784    -0.911988     197.07
 H      -3.422177    -3.366976    -1.900939      25.55
 H      -3.028887    -2.306620     0.942750      19.51
 H      -1.759492    -3.169949    -0.366038      22.38
 C       1.683952    -0.896063    -0.948825      42.45
 H       2.374540    -1.376587    -1.681037      21.54
 C       1.601334     0.729714     0.842539      71.08
 H       2.104099     1.287859     1.649508      21.37
 C       0.235576     0.470452     0.974950      10.77
 O      -0.579701     0.920902     1.933132     173.10
 C       0.145629     1.873913     2.979148     103.36
 H       0.571825     2.619013     2.558378      28.72
 H      -0.531244     2.207270     3.761643      25.96
 H       0.837201     1.050072     3.421644      23.97
 C      -0.445319    -0.324069    -0.078186      14.49
 O      -1.781417    -0.526691     0.142069     161.83
 C       0.344234    -1.186711    -0.852199      77.02
 H       0.162559    -2.062705    -1.617027      19.05
 C       2.367999     0.035677    -0.080773      24.43
 C       3.948304     0.305067    -0.301445      83.50
 H       4.349424     0.146418    -1.292848      19.59
 O       4.074970     1.880444    -0.354129     231.41
 H       4.963003     1.902303    -0.039209      24.62
 C       4.907378    -0.157215     0.851335      77.70
 H       5.028528     0.111970     1.949279      19.81
 O       4.592855    -1.608414     0.688953     308.00
 H       5.207334    -2.250921     1.128503      28.05
 C       6.539759     0.025459     0.326061      68.71
 O       7.116206     1.206057     0.741304     238.83
 H       7.252824     1.016192     1.733751      28.94
 H       6.619194     0.018178    -0.808774      27.70
 H       7.109906    -1.064267     0.737388      25.76
55
name= lig-ACN-Water-frame_828
 C      -4.106181     0.924079    -2.886648      40.41
 H      -4.117405    -0.013746    -3.578933      21.41
 C      -3.730686     2.207230    -0.879326      63.40
 H      -3.410904     2.314798     0.243284      20.96
 C      -3.587209     3.451776    -1.499319       9.15
 O      -3.616917     4.758036    -1.085674     234.20
 C      -3.611528     5.004124     0.335402     105.68
 H      -3.380868     6.274540     0.482679      22.83
 H      -2.717359     4.393999     0.979652      24.18
 H      -4.357589     5.194908     1.085662      25.06
 C      -3.551742     3.314566    -2.937637      10.92
 O      -3.521558     4.419932    -3.713418     177.69
 H      -3.298980     5.146633    -3.002614      20.99
 C      -3.943963     2.160014    -3.624398      56.48
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 H      -3.865733     2.089097    -4.662070      26.91
 C      -4.034282     0.947059    -1.466936      33.41
 C      -4.147181    -0.375001    -0.707222      97.64
 H      -4.827733    -1.105525    -1.157648      24.92
 O      -4.483929    -0.192659     0.607606     276.92
 H      -3.696015     0.069132     1.201446      22.74
 C      -2.683051    -1.177652    -0.820464      74.40
 H      -2.327917    -1.110851    -1.943472      22.45
 C      -2.821594    -2.661025    -0.318076      98.30
 O      -3.742671    -3.554396    -0.874316     264.45
 H      -3.750687    -3.595275    -1.804878      33.03
 H      -3.021805    -2.928565     0.978500      21.53
 H      -1.803888    -3.031221    -0.515955      24.98
 C       1.733761    -0.862815    -0.928306      43.77
 H       2.324012    -1.514408    -1.617131      21.86
 C       1.705422     0.660103     1.001223      67.03
 H       2.248357     1.537090     1.452549      17.96
 C       0.271594     0.393113     0.961968     -16.03
 O      -0.626734     1.097978     2.015234     165.54
 C       0.145894     1.813702     2.911136     116.96
 H       0.585585     2.589825     2.493777      27.91
 H      -0.408755     2.340584     3.840310      24.52
 H       1.058726     1.229944     3.362540      24.18
 C      -0.442416    -0.362596    -0.047867       2.77
 O      -1.831601    -0.622438     0.119334     198.43
 C       0.298451    -1.129156    -0.935194      69.07
 H      -0.381987    -1.697763    -1.549966      17.74
 C       2.414240     0.071593    -0.131655      14.07
 C       3.950561     0.368757    -0.327843      84.25
 H       4.218430    -0.293816    -1.178230      22.94
 O       4.118342     1.843378    -0.314279     203.29
 H       5.007314     2.217424    -0.042687      21.27
 C       4.994270    -0.143538     0.774208      72.58
 H       4.615974     0.381138     1.685573      22.27
 O       4.615013    -1.607894     0.697350     295.30
 H       5.262740    -2.041854     1.309613      27.19
 C       6.524029     0.011003     0.268256      72.48
 O       7.155392     1.240615     0.766837     303.46
 H       7.338539     1.306926     1.705328      32.89
 H       6.632808    -0.040126    -0.872772      27.11
 H       7.201382    -0.937031     0.816582      24.43
55
name= lig-ACN-Water-frame_829
 C      -4.103943     1.006023    -2.871216      65.90
 H      -4.221902     0.017108    -3.334639      24.00
 C      -3.845742     2.226606    -0.842608      51.11
 H      -3.966792     2.156583     0.240445      21.55
 C      -3.631027     3.435728    -1.614529      -8.27
 O      -3.602094     4.754973    -1.017832     226.24
 C      -3.437600     5.061012     0.385117      68.05
 H      -3.035539     6.296031     0.361731      20.13
 H      -2.616414     4.236055     0.944866      22.71
 H      -4.442755     4.601170     0.534710      21.45
 C      -3.571835     3.352685    -3.028464       7.41
 O      -3.464614     4.584854    -3.723576     167.28
 H      -3.434541     5.449614    -3.055711      19.12
 C      -3.956083     2.145218    -3.687721      63.83
 H      -4.061269     2.145308    -4.671257      26.04
 C      -4.089844     1.012808    -1.512532      34.47
 C      -4.085836    -0.358479    -0.755365      89.03
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 H      -4.956927    -0.876272    -1.281875      23.35
 O      -4.517818    -0.225574     0.650558     183.67
 H      -3.688110    -0.108927     1.308575      20.31
 C      -2.800341    -1.244284    -0.769518      66.04
 H      -2.329550    -1.216687    -1.808266      22.49
 C      -2.735475    -2.753874    -0.326869      96.95
 O      -3.788110    -3.570055    -0.919867     254.91
 H      -3.417406    -3.548084    -1.762925      33.08
 H      -3.052208    -2.496821     0.951429      20.59
 H      -1.763185    -3.188001    -0.424802      25.01
 C       1.788125    -0.893776    -1.005824      27.30
 H       2.348930    -1.326807    -1.877665      21.39
 C       1.657526     0.579505     0.944884      50.49
 H       1.998318     1.319195     1.719921      19.65
 C       0.208342     0.473342     1.070989      10.19
 O      -0.606035     1.129606     1.945525     199.54
 C       0.242269     1.894930     2.909292     108.92
 H       0.555899     2.705653     2.508752      27.51
 H      -0.698488     2.028817     3.611541      23.39
 H       0.988857     1.216978     3.523459      23.88
 C      -0.447625    -0.459438     0.140386       8.20
 O      -1.793092    -0.558260     0.201751     151.95
 C       0.376831    -0.974888    -1.000668      72.46
 H       0.115647    -1.625106    -1.697042      22.95
 C       2.480795     0.045010    -0.084805      29.31
 C       3.952922     0.408213    -0.290433     103.42
 H       4.188424     0.255076    -1.406384      24.17
 O       4.132634     1.835935    -0.332232     200.72
 H       5.080977     1.891347     0.029990      23.20
 C       4.986433    -0.261058     0.571569      93.86
 H       4.979489     0.248786     1.621914      19.84
 O       4.664226    -1.549733     0.748569     290.19
 H       5.155963    -2.211797     1.358151      25.42
 C       6.455047     0.015352     0.345839      61.31
 O       7.179632     1.321471     0.753579     262.25
 H       7.052111     1.278088     1.718566      30.44
 H       6.618315     0.048968    -0.794999      23.69
 H       7.075342    -1.047316     0.737590      24.55
55
name= lig-ACN-Water-frame_830
 C      -4.097644     0.995336    -2.988506      57.62
 H      -4.436805     0.138022    -3.435522      25.20
 C      -3.974589     2.331536    -0.752756      66.48
 H      -4.192626     2.503154     0.203732      21.26
 C      -3.698014     3.396968    -1.583570       4.41
 O      -3.508317     4.711982    -1.125617     169.82
 C      -3.373252     4.944798     0.416988      76.86
 H      -3.273614     6.271911     0.558901      23.75
 H      -2.251509     4.419688     0.814103      22.99
 H      -4.138828     4.957417     1.299259      23.82
 C      -3.714429     3.511055    -3.079842       0.31
 O      -3.410740     4.716244    -3.753273     149.05
 H      -3.414735     5.379134    -3.026042      24.18
 C      -3.893737     2.217318    -3.730634      51.30
 H      -4.044704     2.153219    -4.734904      21.88
 C      -4.001972     1.068809    -1.507894      -5.38
 C      -4.066061    -0.405875    -0.667030      80.42
 H      -4.805815    -1.123361    -1.256839      23.97
 O      -4.590312    -0.263977     0.668628     199.14
 H      -3.867866    -0.259300     1.323517      25.94
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 C      -2.723308    -1.264574    -0.779144      74.36
 H      -2.331147    -1.136197    -1.784269      25.08
 C      -2.740861    -2.701426    -0.231584      85.63
 O      -3.826393    -3.600309    -1.013302     159.99
 H      -3.597474    -3.718855    -2.059161      26.91
 H      -2.986709    -2.992371     1.071011      21.84
 H      -1.818992    -3.127252    -0.435401      25.97
 C       1.861934    -0.745511    -1.059364      44.31
 H       2.388325    -1.099417    -1.976786      24.51
 C       1.580170     0.575717     0.900319      60.87
 H       2.259126     0.996864     1.639862      22.98
 C       0.245006     0.382079     0.989428      21.23
 O      -0.497637     1.147402     1.900686     180.40
 C       0.142881     1.994491     2.980272     115.79
 H       0.683116     2.665597     2.629804      29.67
 H      -0.442678     2.526310     3.844136      24.68
 H       0.910925     1.209883     3.358616      24.64
 C      -0.355531    -0.524879     0.124452       4.49
 O      -1.840330    -0.486067     0.295254     101.60
 C       0.458486    -0.944480    -0.926130      66.71
 H      -0.059079    -1.338755    -1.600661      26.07
 C       2.422925    -0.066186    -0.026700       1.76
 C       3.914341     0.367462    -0.402131      76.54
 H       4.075077    -0.140911    -1.443602      22.08
 O       4.195004     1.901598    -0.252511     160.18
 H       4.974436     2.109572     0.252998      21.55
 C       4.992182    -0.174997     0.686559      65.38
 H       4.722976     0.321545     1.686896      20.84
 O       4.631772    -1.653055     0.714250     241.49
 H       5.291397    -1.947088     1.442794      25.37
 C       6.570192     0.070367     0.238233      67.90
 O       7.054528     1.300506     0.737071     284.01
 H       7.227418     1.407606     1.736629      26.17
 H       6.925215    -0.076845    -0.848741      23.88
 H       7.160262    -0.804693     0.999851      24.75
55
name= lig-ACN-Water-frame_831
 C      -4.032265     1.102389    -2.927489      47.69
 H      -4.033186     0.299664    -3.516681      26.45
 C      -4.055591     2.314173    -0.851254      35.46
 H      -3.947166     2.353700     0.127451      22.65
 C      -3.805048     3.555048    -1.639869       9.62
 O      -3.433439     4.728086    -1.052778     169.92
 C      -3.269095     4.913799     0.374560      77.60
 H      -3.120605     6.202845     0.191954      21.20
 H      -2.084752     4.384530     0.637589      23.81
 H      -4.125424     4.338939     0.949631      23.90
 C      -3.796310     3.508036    -3.049213      26.13
 O      -3.419080     4.743277    -3.716515     187.03
 H      -3.249635     5.412704    -3.129476      29.16
 C      -3.896371     2.334734    -3.752419      61.31
 H      -3.716651     2.336130    -4.822998      21.46
 C      -3.983451     0.944711    -1.466962      -7.04
 C      -4.058153    -0.380843    -0.680642      88.36
 H      -4.834407    -1.115885    -1.259696      22.73
 O      -4.635843    -0.313217     0.661019     188.19
 H      -4.004311     0.006156     1.284353      28.08
 C      -2.656926    -1.144694    -0.604263      91.74
 H      -2.246659    -1.207308    -1.567125      25.71
 C      -2.854961    -2.789015    -0.335892      93.79
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 O      -3.790828    -3.549276    -1.015988     228.61
 H      -3.393763    -3.394793    -2.079420      24.10
 H      -3.268305    -2.832067     0.962652      21.79
 H      -1.878741    -3.179911    -0.381835      25.19
 C       1.769128    -0.677839    -1.128126      31.22
 H       2.346835    -0.982258    -2.041340      25.80
 C       1.781740     0.577077     0.985782      43.83
 H       2.002724     1.385563     1.642136      22.98
 C       0.325913     0.387734     1.056194     -11.29
 O      -0.492196     1.204977     1.944064     168.78
 C       0.165141     1.974141     2.945321     124.87
 H       0.610877     2.683296     2.561405      30.19
 H      -0.883146     2.318648     3.273449      24.32
 H       0.687015     1.535268     3.882425      26.13
 C      -0.444512    -0.449738     0.110563      -1.56
 O      -1.767931    -0.513298     0.249788     176.90
 C       0.383524    -1.080330    -0.990303      59.14
 H       0.023415    -1.509658    -1.728765      25.00
 C       2.543962     0.011914    -0.119026      19.44
 C       3.972784     0.369963    -0.243765      99.60
 H       4.354934     0.084515    -1.307255      21.96
 O       4.186252     1.893355    -0.199553     190.50
 H       4.935617     1.881919     0.425919      19.68
 C       4.957135    -0.221031     0.647123      82.08
 H       4.817891     0.299737     1.652748      20.82
 O       4.639330    -1.625805     0.647895     315.70
 H       4.959536    -2.297484     1.268248      28.49
 C       6.591166     0.022029     0.304366      60.00
 O       6.933186     1.381688     0.632133     338.52
 H       7.053103     1.361318     1.673960      25.49
 H       6.573893    -0.082079    -0.823231      25.68
 H       7.321743    -0.919242     0.814987      25.05
55
name= lig-ACN-Water-frame_832
 C      -3.900111     1.126125    -2.947714      57.01
 H      -3.659236     0.250589    -3.381714      24.60
 C      -3.999470     2.293205    -0.952981      62.89
 H      -3.896346     2.291244     0.088232      22.03
 C      -3.934566     3.495041    -1.581286       4.09
 O      -3.391969     4.812471    -1.077915     234.70
 C      -3.129611     4.872059     0.307955      95.77
 H      -3.356675     5.919423     1.085610      22.47
 H      -2.068298     4.283487     0.821589      23.46
 H      -4.004174     4.377913     0.927991      23.02
 C      -3.789115     3.630839    -3.003934       6.18
 O      -3.476908     4.700996    -3.692858     171.31
 H      -3.284021     5.434363    -2.937063      20.11
 C      -3.913020     2.323813    -3.623959      50.48
 H      -3.644528     2.174632    -4.754800      23.75
 C      -4.071560     1.064012    -1.560577      30.66
 C      -4.004494    -0.342233    -0.688953      86.07
 H      -4.704652    -1.073355    -1.416439      21.89
 O      -4.631478    -0.317997     0.625045     204.20
 H      -4.022975     0.226775     1.265094      23.05
 C      -2.705816    -1.187318    -0.655262      75.90
 H      -2.359401    -1.009870    -1.614424      22.62
 C      -2.850704    -2.722705    -0.265620      86.36
 O      -3.783295    -3.459203    -1.114649     299.20
 H      -3.544946    -3.526881    -2.146549      26.68
 H      -3.389508    -2.770078     0.974289      19.70
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 H      -1.899571    -3.233427    -0.219089      24.03
 C       1.707920    -0.671117    -1.108028      41.40
 H       2.177160    -1.081421    -2.042485      20.81
 C       1.812508     0.571898     1.018167      60.18
 H       2.482394     1.198125     1.543370      16.81
 C       0.422486     0.425369     1.091707      14.46
 O      -0.425604     1.086737     1.914084     198.17
 C       0.045034     2.063012     2.945070     114.22
 H       0.693664     2.619922     2.605059      29.34
 H      -0.706185     2.718971     3.436373      25.44
 H       0.577547     1.338522     3.675978      24.90
 C      -0.290320    -0.377594     0.057570      -4.07
 O      -1.717354    -0.524689     0.312737     135.26
 C       0.330648    -1.058486    -1.002902      58.70
 H      -0.042506    -1.783071    -1.474149      21.02
 C       2.470408     0.145306    -0.168187      -4.58
 C       4.081344     0.472281    -0.271691      85.81
 H       4.375635     0.113436    -1.327558      22.94
 O       4.154057     1.832813    -0.104669     223.09
 H       5.066000     2.227158     0.147791      17.28
 C       5.090894    -0.359497     0.777460      89.48
 H       4.981185    -0.140915     1.880465      22.96
 O       4.616792    -1.661370     0.540448     319.23
 H       5.091977    -2.033096     1.306531      27.32
 C       6.406616    -0.024079     0.304336      88.69
 O       6.820758     1.452081     0.484025     273.80
 H       7.081808     1.668063     1.475257      26.57
 H       6.631776    -0.117910    -0.778339      27.28
 H       7.300035    -0.740339     0.882529      26.08
55
name= lig-ACN-Water-frame_833
 C      -3.807400     1.003682    -2.984141      60.64
 H      -3.760314     0.201277    -3.702252      23.38
 C      -3.954620     2.354353    -0.796260      36.45
 H      -4.069940     2.366099     0.346453      21.09
 C      -3.866704     3.671570    -1.556571      -2.39
 O      -3.404722     4.839402    -1.119522     169.77
 C      -3.113097     4.779837     0.484834      60.89
 H      -2.942953     6.077969     0.431723      20.64
 H      -1.896304     4.354103     0.314406      22.09
 H      -3.817607     4.096083     1.025301      20.81
 C      -3.868183     3.495137    -2.947663       8.28
 O      -3.538849     4.746886    -3.684726      89.49
 H      -3.427603     5.609460    -3.017194      20.58
 C      -3.839050     2.326044    -3.628152      47.44
 H      -3.790360     2.502721    -4.847388      21.17
 C      -4.055048     1.046797    -1.558667       9.41
 C      -4.012106    -0.289611    -0.753757      81.62
 H      -4.826442    -1.109117    -1.255561      20.47
 O      -4.588993    -0.256436     0.558314     185.59
 H      -3.939044     0.094954     1.277124      22.94
 C      -2.641905    -1.174600    -0.772653      50.25
 H      -2.189555    -1.362821    -1.700943      21.17
 C      -2.852740    -2.593786    -0.226858      79.45
 O      -3.800877    -3.362785    -1.201408     288.26
 H      -3.299801    -3.348793    -1.981930      30.35
 H      -3.448187    -2.716896     0.930898      20.44
 H      -1.814178    -3.003777    -0.136715      23.25
 C       1.811122    -0.677071    -1.136736      53.56
 H       2.492240    -1.183341    -1.872492      21.56
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 C       1.850151     0.622470     0.967868      64.09
 H       2.249578     0.832504     1.935589      22.82
 C       0.441918     0.459309     1.009559      13.81
 O      -0.450716     1.025168     1.954872     193.15
 C       0.033412     2.043757     2.922441     116.00
 H       0.725703     2.566425     2.519603      30.18
 H      -0.851639     2.600515     3.162528      25.45
 H       0.398083     1.532933     3.892517      24.63
 C      -0.322646    -0.323710     0.159500       8.15
 O      -1.658559    -0.519419     0.401040     104.00
 C       0.434553    -0.972597    -0.931530      62.36
 H      -0.127546    -1.636696    -1.461836      20.20
 C       2.456160     0.128103    -0.238165      25.30
 C       3.994889     0.387289    -0.254802      74.01
 H       4.466082     0.032448    -1.223065      20.75
 O       4.147789     1.942455    -0.018337     236.04
 H       5.110172     1.984038    -0.244304      18.06
 C       4.934740    -0.306376     0.797513      76.71
 H       4.785598    -0.017583     1.825685      23.07
 O       4.673513    -1.833256     0.492590     305.32
 H       4.895695    -2.649405     1.053462      29.06
 C       6.492230     0.021824     0.261720      78.68
 O       6.688235     1.465413     0.320031     265.58
 H       6.945995     1.477497     1.365958      22.30
 H       6.499874    -0.473959    -0.710559      28.75
 H       7.304403    -0.496076     1.050462      26.89
55
name= lig-ACN-Water-frame_834
 C      -3.834150     1.075607    -2.967540      48.55
 H      -3.961221    -0.008879    -3.320610      23.08
 C      -3.972958     2.352401    -0.823523      69.99
 H      -4.091201     2.289572     0.385123      19.90
 C      -3.732738     3.516854    -1.503069       6.83
 O      -3.471304     4.864094    -0.939623     221.91
 C      -2.991056     4.817062     0.344199      99.56
 H      -3.000143     6.008043     1.014802      23.36
 H      -1.931832     4.066413     0.669915      23.43
 H      -3.842526     4.452542     1.010801      25.17
 C      -3.846281     3.582467    -2.959835      -1.77
 O      -3.660590     4.713398    -3.679170     146.42
 H      -3.580063     5.455127    -3.041100      26.13
 C      -3.767056     2.244135    -3.691801      30.04
 H      -3.742521     2.276089    -4.953832      18.90
 C      -3.874858     1.120341    -1.490355      20.07
 C      -3.979688    -0.289090    -0.845493      79.73
 H      -4.726400    -0.985426    -1.603587      22.49
 O      -4.537452    -0.166261     0.520820     181.68
 H      -3.827592     0.018409     1.095623      28.28
 C      -2.593286    -1.085108    -0.707032      75.77
 H      -1.994668    -0.865095    -1.584571      24.95
 C      -2.931385    -2.543847    -0.319029      99.37
 O      -3.719909    -3.204126    -1.175229     344.59
 H      -3.422643    -3.341681    -2.008816      32.71
 H      -3.546934    -2.369878     0.797949      22.41
 H      -2.014453    -3.237900    -0.080196      24.12
 C       1.900373    -0.698473    -1.146983      35.87
 H       2.314936    -1.255671    -2.034976      24.08
 C       1.755621     0.625020     0.914316      79.43
 H       2.419981     1.121105     1.657729      24.43
 C       0.359413     0.564293     1.057070      15.49
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 O      -0.441973     0.981901     2.052521     232.16
 C       0.005211     2.002866     2.892673     133.39
 H       0.680707     2.550896     2.434257      29.08
 H      -0.795392     2.654338     2.964587      27.68
 H       0.322943     1.754457     3.919006      27.11
 C      -0.311382    -0.357496     0.100650       0.48
 O      -1.693239    -0.545609     0.368837     154.33
 C       0.504056    -0.943754    -0.875507      61.80
 H       0.221474    -1.560333    -1.695044      23.94
 C       2.541596     0.104291    -0.123543      23.61
 C       3.947453     0.357084    -0.211996     105.21
 H       4.162522     0.378065    -1.269239      21.97
 O       4.148086     1.962011    -0.020169     206.08
 H       5.105124     2.051281     0.030825      18.33
 C       4.856440    -0.425346     0.682709      97.79
 H       4.579429    -0.168162     1.666022      25.72
 O       4.727129    -1.901434     0.443943     287.61
 H       5.155178    -1.971407     1.357091      26.58
 C       6.418568    -0.019202     0.326544      88.46
 O       6.635541     1.443367     0.185240     200.73
 H       6.765203     1.931470     1.092162      23.24
 H       6.699890    -0.237434    -0.696118      26.50
 H       7.270488    -0.489616     1.052744      26.12
55
name= lig-ACN-Water-frame_835
 C      -3.870024     1.170345    -2.852381      54.97
 H      -3.840191     0.195178    -3.544079      22.77
 C      -3.900407     2.292041    -0.817574      44.76
 H      -3.966514     2.388265     0.419708      17.18
 C      -3.651155     3.505305    -1.567764      -3.57
 O      -3.562100     4.808392    -0.885197     164.48
 C      -2.970436     4.846048     0.474442      71.19
 H      -2.453836     6.158644     0.609280      21.76
 H      -1.864641     4.020425     0.426268      20.43
 H      -3.632622     4.452005     1.252393      24.93
 C      -3.670695     3.460989    -2.988999      37.56
 O      -3.805709     4.720843    -3.678229     190.07
 H      -3.547279     5.386217    -3.122892      29.79
 C      -3.771096     2.323401    -3.655296      72.13
 H      -3.702690     2.071325    -4.852621      22.87
 C      -3.754137     1.100988    -1.525959      39.15
 C      -3.843670    -0.179858    -0.790390     103.83
 H      -4.566247    -0.983334    -1.449295      22.98
 O      -4.522130    -0.099558     0.434845     225.47
 H      -3.899378     0.086674     1.200865      25.29
 C      -2.543352    -0.984624    -0.696546      94.67
 H      -2.144229    -1.015581    -1.760478      22.01
 C      -2.863041    -2.441219    -0.306613      82.18
 O      -3.801833    -3.134889    -1.237733     284.91
 H      -3.262975    -3.205280    -2.113203      27.90
 H      -3.605391    -2.403752     0.729172      21.88
 H      -1.839603    -2.944233     0.037106      23.89
 C       1.872136    -0.703762    -1.013073      57.08
 H       2.532960    -0.906254    -1.876809      23.40
 C       1.682557     0.705020     0.962601      48.99
 H       2.082022     1.650342     1.440225      19.17
 C       0.291899     0.455261     1.004831      12.14
 O      -0.469034     0.897476     2.143893     199.52
 C      -0.019280     2.150256     2.933304     123.48
 H       0.843579     2.496697     2.511933      26.61
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 H      -0.740222     2.793386     3.209374      27.21
 H       0.369819     1.605512     3.724152      26.98
 C      -0.295695    -0.348097     0.067031       4.91
 O      -1.717363    -0.541957     0.324911     199.46
 C       0.525027    -0.994165    -0.991755      64.73
 H      -0.173279    -1.732642    -1.488651      17.61
 C       2.449119     0.032178    -0.058411      17.13
 C       4.014112     0.521350    -0.335993     104.29
 H       4.308127     0.126285    -1.276515      23.54
 O       4.113254     1.868223    -0.012564     243.09
 H       5.076947     2.036619     0.161365      19.44
 C       4.950882    -0.470636     0.571825     113.99
 H       4.732364    -0.264823     1.549874      25.52
 O       4.819966    -1.892322     0.470251     323.84
 H       5.138095    -2.497279     1.097514      31.06
 C       6.309843    -0.057539     0.344144      95.70
 O       6.625827     1.456015     0.121283     292.68
 H       7.026447     1.582297     1.008445      27.87
 H       6.620923    -0.695716    -0.518025      27.39
 H       6.920337    -0.402078     1.270954      27.21
55
name= lig-ACN-Water-frame_836
 C      -3.808086     1.081144    -2.968584      49.10
 H      -3.883563     0.027554    -3.554711      22.51
 C      -3.666576     2.373926    -0.814237      57.95
 H      -3.836193     2.358934     0.384772      19.11
 C      -3.624109     3.553686    -1.503970       9.19
 O      -3.671178     4.713087    -0.900618     160.80
 C      -2.913125     4.810159     0.542789      54.17
 H      -2.788648     6.187977     0.414824      21.82
 H      -1.762953     4.072532     0.421199      19.84
 H      -3.531561     4.677622     1.446658      22.68
 C      -3.536950     3.594918    -2.947352       5.85
 O      -3.905722     4.721264    -3.678616     162.95
 H      -3.652921     5.553284    -3.096531      23.84
 C      -3.781966     2.327961    -3.658149      21.97
 H      -3.921488     2.549386    -4.797011      21.25
 C      -3.760943     1.148829    -1.473881      16.36
 C      -3.765846    -0.175560    -0.744603      94.56
 H      -4.512475    -0.876058    -1.488703      19.46
 O      -4.554908    -0.024803     0.457610     228.45
 H      -3.958028     0.210016     1.322904      21.55
 C      -2.545198    -1.036120    -0.778970      67.20
 H      -1.943906    -1.033371    -1.771734      18.40
 C      -2.888655    -2.400186    -0.282662      89.61
 O      -3.827316    -3.067895    -1.271677     253.40
 H      -3.394256    -3.301746    -2.296083      23.50
 H      -3.336844    -2.375450     0.860229      20.82
 H      -1.908077    -3.097534    -0.404318      19.63
 C       1.823072    -0.792975    -0.989831      23.70
 H       2.433602    -1.307660    -1.759356      21.28
 C       1.656220     0.798323     0.944721      67.41
 H       2.058748     1.523688     1.743110      20.79
 C       0.322038     0.412699     1.125396       1.51
 O      -0.530010     0.900432     2.179332     166.49
 C       0.042631     2.115161     2.997705     120.57
 H       0.581153     2.868089     2.406802      26.15
 H      -0.825343     2.588008     2.920693      27.62
 H       0.337979     2.051081     3.950315      27.27
 C      -0.356699    -0.414466     0.033276      24.97
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 O      -1.617616    -0.466095     0.285706     168.90
 C       0.330533    -1.040580    -0.998057      58.98
 H       0.148627    -1.822097    -1.898376      17.60
 C       2.502591     0.194468    -0.008766      33.72
 C       3.873551     0.366215    -0.371589     113.01
 H       3.949079     0.438467    -1.417405      21.23
 O       4.090113     1.815243    -0.003522     249.53
 H       5.106001     1.909720     0.010446      19.78
 C       4.902331    -0.342004     0.671899      87.60
 H       4.633024     0.034958     1.570101      25.20
 O       4.865760    -1.913227     0.376901     261.08
 H       5.176590    -2.151876     1.295476      28.23
 C       6.477310    -0.093735     0.308163      98.74
 O       6.640723     1.361401     0.143447     298.39
 H       7.308665     1.663138     0.737648      31.94
 H       6.971570    -0.638496    -0.526338      26.64
 H       7.032660    -0.297384     1.256968      26.56
55
name= lig-ACN-Water-frame_837
 C      -3.723887     1.113907    -2.966283      60.08
 H      -4.056800     0.077807    -3.392843      22.17
 C      -3.458856     2.339628    -0.832525      47.93
 H      -3.472128     2.379254     0.298462      20.21
 C      -3.542217     3.558724    -1.511071      -4.06
 O      -3.714733     4.783882    -0.728321     280.09
 C      -2.974518     4.859574     0.408456      92.91
 H      -2.677754     6.128307     0.841718      20.57
 H      -1.767079     4.183499     0.557617      20.27
 H      -3.590666     4.308588     1.161063      22.78
 C      -3.626969     3.600815    -2.938335      14.50
 O      -3.940587     4.766889    -3.666818     174.13
 H      -3.882900     5.709954    -3.093954      21.81
 C      -3.728564     2.386990    -3.634512      53.62
 H      -4.046743     2.380847    -4.658819      22.99
 C      -3.700107     1.153015    -1.614575      21.16
 C      -3.906038    -0.153155    -0.812014      70.69
 H      -4.711454    -0.872127    -1.403464      19.78
 O      -4.561679     0.015211     0.545307     212.85
 H      -3.842730     0.263050     1.222839      22.53
 C      -2.505520    -1.037092    -0.696262      71.36
 H      -2.141755    -0.912567    -1.818438      19.26
 C      -2.880480    -2.558645    -0.424842     100.95
 O      -3.877930    -2.989767    -1.222590     303.27
 H      -3.316299    -3.183964    -2.163969      23.88
 H      -3.398875    -2.565392     0.653324      21.78
 H      -1.873203    -3.251880    -0.220340      21.80
 C       1.718939    -0.807151    -0.893816      74.65
 H       2.353094    -1.431521    -1.493117      21.63
 C       1.669351     0.812048     0.973720      76.89
 H       2.384995     1.296079     1.696393      21.35
 C       0.353919     0.396737     1.182131       4.07
 O      -0.451237     0.929747     2.199885     215.66
 C      -0.105428     2.089665     2.936308     115.01
 H       0.807296     2.536135     2.330460      22.84
 H      -0.882002     2.624841     3.324542      26.51
 H       0.408913     1.705707     3.695588      27.40
 C      -0.281092    -0.410484     0.146314       4.80
 O      -1.722487    -0.415371     0.234356     189.55
 C       0.446219    -1.030038    -0.935610      64.28
 H      -0.333672    -1.569903    -1.754193      16.54
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 C       2.263851     0.103376    -0.163087      34.70
 C       3.864253     0.355652    -0.274571      91.70
 H       4.198662    -0.182856    -1.149591      22.34
 O       4.077469     1.815296    -0.031267     249.36
 H       5.087214     1.949660    -0.039649      17.62
 C       4.947063    -0.391120     0.525200     120.66
 H       4.721100    -0.306422     1.490538      25.74
 O       4.873541    -1.803454     0.389298     295.73
 H       5.054930    -2.278391     1.299071      27.79
 C       6.559518    -0.079859     0.372211      92.98
 O       6.748849     1.309430     0.125440     310.54
 H       6.991799     1.687557     1.100614      23.95
 H       6.667666    -0.558968    -0.618224      27.67
 H       7.162400    -0.581239     1.093883      29.85
55
name= lig-ACN-Water-frame_838
 C      -3.718152     1.202425    -2.968982      43.46
 H      -3.910824     0.431363    -3.759507      21.94
 C      -3.321449     2.287755    -0.908830      45.11
 H      -3.126847     2.169035     0.106266      18.90
 C      -3.478505     3.651701    -1.472656      17.22
 O      -3.739893     4.837154    -0.777232     226.71
 C      -2.996609     4.842120     0.534474      86.31
 H      -2.981201     6.168942     0.831603      22.80
 H      -1.834879     4.514764    -0.043594      20.47
 H      -3.350864     4.285509     1.478166      24.08
 C      -3.804180     3.632170    -2.917271       7.96
 O      -3.959192     4.810445    -3.645302     143.51
 H      -3.648397     5.537744    -2.974150      23.92
 C      -3.696318     2.447053    -3.684627      50.54
 H      -3.743866     2.434285    -4.694895      22.12
 C      -3.568894     1.075632    -1.526968      31.23
 C      -4.000641    -0.183005    -0.766625      91.25
 H      -4.824330    -0.787661    -1.366654      21.12
 O      -4.546378     0.036281     0.515338     253.65
 H      -3.988878     0.375662     1.186871      26.14
 C      -2.670004    -1.054058    -0.731689      64.13
 H      -2.076513    -1.026426    -1.738036      20.34
 C      -2.813861    -2.580773    -0.356518      92.83
 O      -3.964258    -3.009760    -1.300015     261.34
 H      -3.766163    -3.214669    -2.205369      29.36
 H      -3.235389    -2.654703     0.723870      23.71
 H      -1.854308    -3.330769    -0.595629      21.31
 C       1.796089    -0.933161    -1.000219      10.03
 H       2.438403    -1.287036    -1.808157      20.78
 C       1.701517     0.681336     0.973763      80.50
 H       2.173512     1.491707     1.536197      22.10
 C       0.335467     0.464797     1.190641      22.61
 O      -0.494755     0.873727     2.155034     214.00
 C      -0.063643     2.025684     2.936129     118.65
 H       0.355695     3.041107     2.333244      23.29
 H      -0.981413     2.468685     3.265333      25.52
 H       0.454519     1.772469     3.735393      28.00
 C      -0.389703    -0.372215     0.280119      25.96
 O      -1.734722    -0.329877     0.287552     145.45
 C       0.245015    -1.016243    -0.740826      49.58
 H      -0.322217    -1.811273    -1.536210      18.69
 C       2.449042     0.127584    -0.073913       8.81
 C       3.902758     0.355048    -0.279595      96.70
 H       3.962506     0.396407    -1.354690      21.95
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 O       4.064806     1.783669    -0.139329     264.17
 H       5.023362     1.912907    -0.052796      20.72
 C       5.033869    -0.438239     0.726903      95.57
 H       4.915214    -0.082799     1.648813      25.90
 O       4.838496    -1.827052     0.360278     326.94
 H       4.938135    -2.324996     1.156728      30.35
 C       6.433573    -0.130920     0.230964     117.40
 O       6.916326     1.348620     0.183354     298.58
 H       6.956652     1.646543     1.224760      24.80
 H       6.842718    -0.605318    -0.653401      26.31
 H       7.002369    -0.447983     1.040537      27.26
55
name= lig-ACN-Water-frame_839
 C      -3.726242     1.204544    -3.014519      54.13
 H      -3.659330     0.213572    -3.414806      21.48
 C      -3.222531     2.387743    -0.872071      44.96
 H      -3.009775     2.446674     0.084475      20.71
 C      -3.557291     3.563261    -1.525326      16.42
 O      -3.735575     4.800897    -0.822096     166.32
 C      -2.955369     4.909630     0.565119      77.51
 H      -3.366739     6.060578     1.031877      23.90
 H      -1.602329     4.873174     0.735181      21.65
 H      -3.381941     4.022020     1.210335      23.65
 C      -3.834276     3.715101    -2.880035      27.29
 O      -3.990330     4.876709    -3.584468     231.00
 H      -3.594032     5.663950    -3.190579      28.19
 C      -3.706250     2.508524    -3.649822      45.08
 H      -3.577915     2.679481    -4.644856      22.64
 C      -3.536673     1.131260    -1.612371       7.33
 C      -3.887902    -0.225838    -0.749412      90.74
 H      -4.659198    -0.686511    -1.420934      22.56
 O      -4.622619     0.042143     0.464070     239.11
 H      -3.997106     0.344244     1.166984      24.14
 C      -2.730993    -1.121647    -0.694905      71.55
 H      -2.313576    -0.968652    -1.757640      19.98
 C      -2.914892    -2.564616    -0.422279     109.17
 O      -4.025774    -3.056948    -1.297520     304.92
 H      -3.507288    -3.204153    -2.004701      32.65
 H      -3.013656    -2.877812     0.574298      26.68
 H      -1.853723    -3.032368    -0.847710      20.69
 C       1.696230    -0.814915    -0.892431      64.02
 H       1.860144    -1.303347    -1.822663      23.08
 C       1.729250     0.623858     1.018675      46.00
 H       2.143082     1.378008     1.640814      20.98
 C       0.298149     0.420144     1.105971       0.82
 O      -0.540031     0.914575     2.174884     182.72
 C      -0.097995     2.034757     3.009882     100.35
 H       0.232979     2.851465     2.117440      22.19
 H      -1.045800     2.241459     3.541844      23.96
 H       0.669392     1.921319     3.660701      27.23
 C      -0.450580    -0.382248     0.221163       0.47
 O      -1.887020    -0.271264     0.395363     100.98
 C       0.398604    -1.103333    -0.670607      59.95
 H      -0.193269    -1.945575    -1.311495      18.37
 C       2.529882    -0.140905    -0.080427      23.71
 C       3.994164     0.364744    -0.322250      91.27
 H       4.439976    -0.263350    -1.134386      22.94
 O       4.102786     1.838362    -0.208875     238.56
 H       5.045953     2.065249    -0.092381      23.68
 C       4.947682    -0.325554     0.671476      95.47
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 H       4.788531    -0.263751     1.660627      26.45
 O       4.788653    -1.915879     0.387587     237.37
 H       4.938144    -2.403455     1.221602      29.53
 C       6.529350    -0.088098     0.208588      97.02
 O       6.944993     1.301804     0.232411     247.79
 H       7.570694     1.384808     1.023243      26.79
 H       6.504269    -0.419103    -0.822019      28.68
 H       7.154614    -0.733558     0.729017      28.20
55
name= lig-ACN-Water-frame_840
 C      -3.668238     1.230270    -2.990709      57.50
 H      -3.843830     0.494489    -3.686965      23.84
 C      -3.244649     2.363095    -0.872426      60.21
 H      -3.053959     2.253167     0.117467      22.58
 C      -3.644690     3.643270    -1.459496       0.18
 O      -3.571858     4.785198    -0.754117     202.94
 C      -3.085314     4.942116     0.546485      83.43
 H      -3.628125     5.973671     1.026508      22.20
 H      -1.760768     5.048097     0.329332      22.84
 H      -3.391588     3.993116     1.275912      21.71
 C      -3.769454     3.667639    -2.928934      15.96
 O      -4.053736     4.958677    -3.556303     190.97
 H      -3.675661     5.632861    -3.035454      24.76
 C      -3.750901     2.512475    -3.648084      66.64
 H      -3.847435     2.466041    -4.728928      24.37
 C      -3.534083     1.233527    -1.572248      25.38
 C      -3.907715    -0.079701    -0.894217      98.39
 H      -4.533078    -0.689400    -1.511047      23.82
 O      -4.695302     0.049093     0.390686     210.30
 H      -4.109663     0.004527     1.268989      22.75
 C      -2.665065    -0.998834    -0.596209      80.67
 H      -1.968645    -0.984523    -1.475179      22.23
 C      -2.985081    -2.641218    -0.496330     113.11
 O      -4.018076    -3.117533    -1.269251     288.34
 H      -3.918943    -3.412610    -2.248522      28.55
 H      -3.305421    -2.794191     0.449213      26.51
 H      -1.974889    -3.308281    -0.701587      22.51
 C       1.699186    -0.841625    -0.903289      25.40
 H       2.402670    -1.271646    -1.595499      22.92
 C       1.732192     0.497299     1.015912      71.86
 H       2.317092     0.902722     1.784674      22.96
 C       0.298574     0.420839     1.160101       8.14
 O      -0.503839     0.933803     2.176371     216.30
 C      -0.155299     2.060998     3.002956     108.64
 H       0.043377     3.229886     2.517110      22.33
 H      -0.796568     2.366366     3.892581      24.77
 H       0.688843     1.723431     3.373896      27.87
 C      -0.507995    -0.373144     0.211135       5.54
 O      -1.907527    -0.399421     0.378986     211.55
 C       0.271991    -1.225342    -0.645186      61.87
 H      -0.046385    -1.918892    -1.465297      20.70
 C       2.472627    -0.070782     0.061172      18.59
 C       4.008058     0.242210    -0.325823      70.69
 H       4.068588     0.186197    -1.473166      22.79
 O       4.153408     1.839277    -0.319875     185.72
 H       5.102254     1.971179     0.008853      21.28
 C       5.030562    -0.429088     0.636378     103.48
 H       4.697060    -0.025472     1.583159      25.31
 O       4.754310    -1.866014     0.438677     259.00
 H       5.010704    -2.135512     1.412942      27.30
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 C       6.505959    -0.121970     0.216012     113.82
 O       6.969772     1.227788     0.277025     317.72
 H       7.155067     1.542425     1.198362      27.75
 H       6.441367    -0.238622    -0.844459      27.05
 H       7.252650    -0.737275     0.463504      28.84
55
name= lig-ACN-Water-frame_841
 C      -3.659427     1.317502    -3.013933      60.50
 H      -3.937969     0.376788    -3.339263      24.81
 C      -3.391300     2.417667    -0.835016      67.18
 H      -3.267805     2.356905     0.253238      21.53
 C      -3.541157     3.624994    -1.449328      11.05
 O      -3.506395     4.882934    -0.812512     200.54
 C      -3.187505     4.930142     0.605835      95.18
 H      -3.619547     5.984589     0.971147      23.34
 H      -1.820506     5.182884     0.728903      22.88
 H      -3.320513     4.051392     1.446727      22.44
 C      -3.762323     3.772953    -2.875134     -14.05
 O      -4.127102     4.908449    -3.525124     257.84
 H      -3.567789     5.666382    -3.217182      25.18
 C      -3.777443     2.502533    -3.690366      17.83
 H      -4.159836     2.525265    -4.788951      19.46
 C      -3.573205     1.199458    -1.605118      12.45
 C      -3.925985    -0.086995    -0.909898     102.28
 H      -4.521361    -0.535371    -1.613254      26.03
 O      -4.732670     0.066526     0.252953     189.70
 H      -4.056177     0.045793     1.056463      24.08
 C      -2.620927    -1.014809    -0.769904      55.11
 H      -2.134699    -0.826410    -1.720968      22.99
 C      -2.991565    -2.608947    -0.425087      93.52
 O      -4.118320    -3.199745    -1.312670     260.69
 H      -3.474260    -3.144575    -2.239880      24.70
 H      -3.279226    -2.669288     0.498321      27.66
 H      -1.987362    -3.254937    -0.476716      22.03
 C       1.723127    -0.976093    -0.841452      40.01
 H       2.127701    -1.456518    -1.747303      23.35
 C       1.661633     0.477234     1.249839      51.18
 H       2.062691     1.076419     2.056062      20.17
 C       0.256740     0.401190     1.198720      11.82
 O      -0.547420     0.977600     2.173456     174.18
 C      -0.024722     2.095937     3.020693      94.85
 H      -0.182822     3.041322     2.209869      22.14
 H      -1.040583     1.964634     3.603921      21.88
 H       0.855716     2.180305     3.565612      25.76
 C      -0.409350    -0.436173     0.255781       4.70
 O      -1.786914    -0.544847     0.456233     161.22
 C       0.268946    -1.191034    -0.744392      65.18
 H      -0.334942    -1.849706    -1.233409      21.32
 C       2.396777    -0.013363    -0.024367      17.17
 C       3.822894     0.311166    -0.353888      71.46
 H       3.912095    -0.206663    -1.439715      23.73
 O       4.198855     1.732812    -0.371340     201.09
 H       5.159874     1.823685    -0.099562      21.31
 C       5.063351    -0.459561     0.597860      83.50
 H       5.110086    -0.118018     1.655330      23.01
 O       4.762116    -1.817510     0.572320     309.16
 H       4.972327    -2.436593     1.255842      29.74
 C       6.504962    -0.217541     0.128146     103.43
 O       6.957938     1.228501     0.359916     353.49
 H       6.954626     1.415880     1.294437      30.49
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 H       6.824412    -0.551235    -0.860493      26.50
 H       6.943371    -0.766434     0.814153      29.16
55
name= lig-ACN-Water-frame_842
 C      -3.738289     1.283826    -3.001934      55.23
 H      -3.748555     0.487427    -3.723956      23.06
 C      -3.551558     2.424234    -0.803058      45.61
 H      -3.599385     2.394696     0.377177      18.07
 C      -3.403182     3.708646    -1.521817       3.22
 O      -3.477575     4.945824    -0.848961     141.13
 C      -3.195520     5.010646     0.712251      83.14
 H      -3.792280     5.870830     1.045694      24.36
 H      -1.857653     5.012800     1.131738      19.90
 H      -3.929418     4.124923     0.890390      22.35
 C      -3.765209     3.690727    -2.885886      23.65
 O      -4.175107     4.912831    -3.510915     168.91
 H      -3.645611     5.618787    -3.109608      28.81
 C      -3.831448     2.615629    -3.632367      48.74
 H      -4.043538     2.869458    -4.800080      21.66
 C      -3.600058     1.278854    -1.600209      29.17
 C      -3.862217    -0.206117    -0.976759     108.57
 H      -4.457771    -0.799906    -1.539809      25.85
 O      -4.705426     0.077743     0.176924     183.14
 H      -4.283836     0.353943     0.975294      26.00
 C      -2.696151    -1.136665    -0.848942      61.58
 H      -2.080883    -1.126749    -1.693865      23.08
 C      -3.059213    -2.499141    -0.428284     117.83
 O      -4.057599    -3.184475    -1.311299     288.04
 H      -3.705179    -3.440837    -2.262470      28.85
 H      -3.371625    -2.463527     0.507158      28.07
 H      -2.136585    -3.147263    -0.543165      22.52
 C       1.672473    -1.002684    -0.798660      42.68
 H       2.263327    -1.367194    -1.674422      22.04
 C       1.652140     0.474627     1.217371      69.31
 H       2.262916     1.202827     1.807392      19.20
 C       0.268141     0.335574     1.279523      19.83
 O      -0.552013     0.984486     2.182526     222.71
 C      -0.082807     2.130560     2.973218      95.55
 H       0.122410     3.153626     2.260895      22.96
 H      -0.687906     2.587620     3.909869      22.73
 H       0.869140     1.811379     3.368835      24.74
 C      -0.364037    -0.522024     0.336330       9.48
 O      -1.725360    -0.694585     0.440463     115.09
 C       0.354446    -1.118834    -0.778807      88.96
 H      -0.024237    -1.792020    -1.360881      23.09
 C       2.257062    -0.021575     0.078375      34.92
 C       3.821937     0.258776    -0.319935      87.66
 H       4.163074    -0.235293    -1.356389      22.05
 O       4.192037     1.648175    -0.385991     245.90
 H       5.148129     1.620594    -0.287443      26.41
 C       4.959785    -0.368381     0.542851      71.41
 H       4.854918     0.148594     1.562369      23.57
 O       4.727440    -1.904605     0.643893     253.08
 H       5.263925    -1.990462     1.452841      29.05
 C       6.592122    -0.239353     0.171369     101.29
 O       6.871441     1.160168     0.372381     281.91
 H       7.495532     1.266834     1.188124      26.13
 H       6.892445    -0.566162    -0.840017      27.66
 H       7.112627    -0.759875     0.860971      29.07
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name= lig-ACN-Water-frame_843
 C      -3.782666     1.355042    -3.064781      50.29
 H      -3.701656     0.390413    -3.626182      23.50
 C      -3.613531     2.481076    -0.891001      47.56
 H      -3.684739     2.343058     0.319092      17.84
 C      -3.426409     3.741443    -1.412554      15.14
 O      -3.364182     5.029776    -0.787741     199.18
 C      -3.384081     5.016545     0.631811     105.17
 H      -3.399866     6.001967     0.914306      25.19
 H      -2.051085     4.574220     1.002919      22.00
 H      -3.931961     4.348286     1.370339      25.55
 C      -3.764832     3.820768    -2.850369       4.57
 O      -4.171324     4.936100    -3.493394     179.29
 H      -3.787454     5.673883    -3.126593      28.79
 C      -3.891351     2.549644    -3.629261      60.63
 H      -3.947545     2.508195    -4.855837      23.11
 C      -3.678113     1.181244    -1.644736      21.98
 C      -3.846483    -0.130684    -1.055129     115.65
 H      -4.390599    -0.585974    -1.731589      28.71
 O      -4.665693     0.034971     0.173323     202.99
 H      -4.007318     0.225604     0.847994      26.73
 C      -2.593282    -1.132380    -0.780660      94.96
 H      -2.080248    -1.137567    -1.682660      26.10
 C      -3.111203    -2.596897    -0.453200     121.06
 O      -4.019318    -3.140851    -1.295258     369.28
 H      -3.544776    -3.469125    -1.959348      34.68
 H      -3.643209    -2.415426     0.444937      26.65
 H      -2.204162    -3.142906    -0.186287      27.11
 C       1.775673    -0.873705    -0.843298      28.28
 H       2.486064    -1.414184    -1.547886      22.82
 C       1.678440     0.571830     1.088486      77.13
 H       2.224231     1.308377     1.786852      21.57
 C       0.266464     0.282928     1.375438      -4.96
 O      -0.639690     0.998448     2.234478     187.95
 C      -0.013294     2.133388     2.894501      85.47
 H       0.256465     3.014173     2.061709      22.89
 H      -0.894380     2.328564     3.677796      22.89
 H       0.911868     1.883990     3.490484      24.77
 C      -0.421504    -0.592462     0.336485       2.65
 O      -1.814375    -0.841028     0.364305     212.78
 C       0.305671    -1.176169    -0.715187      50.11
 H      -0.181779    -1.598596    -1.487199      22.82
 C       2.497713    -0.124969     0.127206      26.14
 C       3.886436     0.102994    -0.328305      85.06
 H       3.631004    -0.092743    -1.405783      22.69
 O       4.147241     1.637082    -0.387585     228.68
 H       5.078255     1.872553    -0.146651      24.94
 C       4.933669    -0.482324     0.599789      98.52
 H       4.700974     0.036632     1.573111      25.63
 O       4.727330    -1.876518     0.739528     239.94
 H       5.228308    -2.253327     1.606057      27.99
 C       6.481539    -0.241502     0.273990     101.96
 O       6.854279     1.151217     0.357499     250.69
 H       7.588594     1.417330     1.019281      26.51
 H       6.558690    -0.526339    -0.788989      27.94
 H       7.096488    -0.909925     0.808038      29.13
55
name= lig-ACN-Water-frame_844
 C      -3.770261     1.306292    -3.062782      45.33
 H      -4.035821     0.376968    -3.670981      22.19
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 C      -3.589643     2.431298    -0.897093      64.07
 H      -3.527318     2.311210     0.303156      19.92
 C      -3.604565     3.762207    -1.480510     -10.72
 O      -3.313102     4.992445    -0.781098     120.36
 C      -3.408285     5.056756     0.664588      96.68
 H      -3.305843     5.984511     0.966009      24.63
 H      -2.320988     4.229305     1.245881      20.17
 H      -4.420720     4.726234     0.792374      26.82
 C      -3.784333     3.794991    -2.858474      25.06
 O      -4.154914     5.031335    -3.511487     174.82
 H      -3.500955     5.630332    -3.262199      25.98
 C      -3.885276     2.668117    -3.635766      16.61
 H      -4.158362     2.918596    -4.795912      22.89
 C      -3.712793     1.322912    -1.700038      34.10
 C      -3.863559    -0.143026    -1.016614      98.89
 H      -4.407391    -0.743607    -1.559038      26.79
 O      -4.582127    -0.049891     0.182786     187.06
 H      -4.059036    -0.036128     1.093891      21.07
 C      -2.578446    -1.130599    -0.836712      78.79
 H      -1.891726    -1.022741    -1.630144      24.54
 C      -3.100262    -2.591445    -0.314471      99.32
 O      -4.049377    -3.193832    -1.382644     271.02
 H      -3.568119    -3.352058    -2.225449      28.73
 H      -3.634283    -2.411854     0.678993      24.90
 H      -2.365991    -3.277894    -0.177394      26.75
 C       1.730382    -0.900376    -0.842788      48.75
 H       2.000745    -1.353336    -1.848449      22.47
 C       1.649147     0.614031     1.092994      80.23
 H       2.040333     1.458386     1.749435      20.95
 C       0.214653     0.239421     1.248791       6.42
 O      -0.595460     0.926132     2.199386     206.68
 C       0.014782     2.092531     2.864460     100.95
 H       0.329477     2.873908     1.972826      24.01
 H      -0.817907     2.737682     3.412701      24.34
 H       0.807835     2.009997     3.536293      26.81
 C      -0.416837    -0.606570     0.363718      10.52
 O      -1.857521    -0.859088     0.429323     188.86
 C       0.453200    -1.170463    -0.673507      50.33
 H      -0.068562    -1.811532    -1.408464      22.49
 C       2.487119    -0.170464     0.122983      19.86
 C       3.986709     0.169159    -0.373050      80.83
 H       4.579172    -0.402742    -1.092593      23.47
 O       4.080120     1.598059    -0.378082     240.82
 H       4.956551     1.761664     0.105603      22.50
 C       4.987034    -0.529079     0.769396      92.80
 H       4.808229    -0.018928     1.759538      25.49
 O       4.734698    -1.937009     0.826568     285.42
 H       5.008171    -2.417818     1.640776      29.46
 C       6.336562    -0.263055     0.275198      98.68
 O       6.863453     1.201461     0.346291     253.79
 H       7.102398     1.168262     1.246997      31.18
 H       6.528499    -0.611028    -0.752055      28.07
 H       7.009890    -0.755311     1.028553      26.91
55
name= lig-ACN-Water-frame_845
 C      -3.841089     1.430434    -3.144029      35.19
 H      -4.048851     0.563234    -3.860098      22.25
 C      -3.546782     2.493390    -0.834120      37.48
 H      -3.342443     2.358838     0.301155      17.28
 C      -3.695487     3.742482    -1.451612       2.90
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 O      -3.280457     4.913059    -0.878943     169.91
 C      -3.446837     5.026367     0.685814     114.99
 H      -3.155577     5.939864     0.960361      25.74
 H      -3.149404     4.054032     1.594647      20.01
 H      -4.449551     4.788683     0.923988      28.87
 C      -3.884367     3.869359    -2.914757       6.23
 O      -4.085743     5.084313    -3.548723     209.25
 H      -3.632542     5.851951    -3.209067      26.40
 C      -3.881649     2.693631    -3.695389      50.78
 H      -4.220226     2.844630    -4.808060      19.77
 C      -3.697280     1.221691    -1.651012      -8.13
 C      -3.810000    -0.189838    -1.001052     103.58
 H      -4.395695    -0.606154    -1.662269      26.93
 O      -4.566945    -0.141780     0.278407     184.70
 H      -3.883832     0.166183     1.017622      21.58
 C      -2.652057    -1.185217    -0.789931      52.95
 H      -2.011701    -1.330760    -1.674394      22.60
 C      -3.127185    -2.554928    -0.487503     115.74
 O      -4.057381    -3.221022    -1.361673     244.80
 H      -3.536404    -3.236271    -2.358630      24.98
 H      -3.761771    -2.391221     0.543025      23.46
 H      -2.298733    -3.030233    -0.309223      27.26
 C       1.783505    -0.998018    -0.853730      35.99
 H       2.519396    -1.145912    -1.704460      22.35
 C       1.634545     0.457983     1.029253      74.28
 H       2.167063     1.216708     1.614338      21.33
 C       0.283961     0.360274     1.165532      19.81
 O      -0.475112     0.845482     2.175631     235.48
 C      -0.024564     2.098408     2.766406     106.88
 H       0.631669     2.684202     2.001247      24.20
 H      -0.904403     2.603917     3.282481      23.61
 H       0.544684     1.712761     3.442095      28.25
 C      -0.427307    -0.658553     0.327949      17.71
 O      -1.746658    -0.762773     0.544178     142.84
 C       0.291441    -1.234310    -0.646096      83.70
 H      -0.056560    -2.139255    -1.329366      21.08
 C       2.388402    -0.033389    -0.005536      17.14
 C       3.990328     0.117568    -0.119826      86.07
 H       3.941372    -0.214530    -1.183911      23.22
 O       4.077978     1.578686    -0.359239     254.16
 H       4.910293     1.986231    -0.095134      25.24
 C       4.905038    -0.393021     0.912969      83.19
 H       4.823881    -0.049448     2.020648      23.85
 O       4.728645    -2.039966     0.870623     228.48
 H       5.035583    -2.115011     1.757803      30.30
 C       6.480961    -0.232911     0.340619      81.94
 O       6.806689     1.169140     0.375176     257.13
 H       6.793819     1.625110     1.247811      28.59
 H       6.512855    -0.554525    -0.723948      26.30
 H       7.277668    -0.937344     0.865486      25.48
55
name= lig-ACN-Water-frame_846
 C      -3.915661     1.473160    -3.006759      45.32
 H      -3.842544     0.541765    -3.623018      20.49
 C      -3.551579     2.385370    -0.908963      52.39
 H      -3.284064     2.429689     0.137863      16.78
 C      -3.659717     3.688285    -1.529564       6.15
 O      -3.261174     4.887050    -0.779258     247.05
 C      -3.598607     4.955687     0.606281     100.92
 H      -2.973757     5.785732     0.915093      24.42
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 H      -2.717493     4.069223     0.931584      19.78
 H      -4.554335     5.119307     0.730028      29.17
 C      -3.966298     3.914579    -2.901294       4.26
 O      -4.071063     5.086955    -3.616485     219.29
 H      -3.462191     5.710790    -3.095131      24.28
 C      -3.978241     2.740431    -3.738646      37.30
 H      -3.893148     2.682070    -4.831062      22.51
 C      -3.644907     1.249750    -1.666412      41.14
 C      -3.822531    -0.169671    -0.969037     111.19
 H      -4.378092    -0.761406    -1.531600      27.45
 O      -4.562397    -0.210705     0.305083     191.89
 H      -4.126313     0.201202     1.080443      23.85
 C      -2.621219    -1.107007    -0.743677      68.55
 H      -1.918903    -0.896306    -1.616346      23.60
 C      -3.124693    -2.603207    -0.523309     105.68
 O      -4.062182    -3.215166    -1.382101     266.49
 H      -3.679454    -3.587811    -2.378934      23.61
 H      -3.646309    -2.558392     0.613106      23.94
 H      -2.397848    -3.232533    -0.428115      27.67
 C       1.693138    -1.041523    -0.898803      57.05
 H       2.113989    -1.868391    -1.496931      21.98
 C       1.706682     0.494606     1.049734      38.20
 H       2.204597     0.907366     1.886590      21.81
 C       0.285742     0.299000     1.082406      15.83
 O      -0.451145     0.832665     2.145681     235.37
 C      -0.006417     2.025896     2.756724     135.31
 H       0.480012     2.746704     2.084268      27.09
 H      -0.950998     2.568671     2.966199      25.90
 H       0.463934     2.104094     3.539766      30.43
 C      -0.353966    -0.578011     0.279699      -1.09
 O      -1.787149    -0.720504     0.511269     149.38
 C       0.397755    -1.400017    -0.756569      52.49
 H      -0.433741    -2.139967    -1.298265      17.03
 C       2.363080    -0.078921    -0.074964      43.93
 C       3.777767     0.158498    -0.049523      87.62
 H       4.382970    -0.490834    -0.811389      23.79
 O       4.101485     1.642685    -0.307956     229.46
 H       5.089502     1.586792    -0.336393      24.77
 C       5.006810    -0.534016     0.932855      80.18
 H       4.710381    -0.046684     1.990973      24.35
 O       4.758751    -1.940748     0.966214     252.42
 H       4.994270    -2.534884     1.778650      27.72
 C       6.459413    -0.188694     0.480470      92.05
 O       6.786463     1.211757     0.399841     193.60
 H       6.844626     1.452891     1.421183      25.56
 H       6.421487    -0.454748    -0.603390      27.37
 H       7.307488    -0.839844     1.084994      25.37
55
name= lig-ACN-Water-frame_847
 C      -3.926395     1.367970    -3.032287      52.67
 H      -4.069103     0.528429    -3.717870      22.68
 C      -3.518961     2.436773    -0.928221      55.76
 H      -3.396901     2.327377     0.119043      19.58
 C      -3.574934     3.742987    -1.548241      16.97
 O      -3.301211     4.847530    -0.848994     250.98
 C      -3.558482     4.883077     0.561839     137.71
 H      -3.388557     5.870237     1.051451      26.63
 H      -3.642364     4.008920     1.398802      21.71
 H      -4.549336     4.722573     0.676070      28.60
 C      -3.973467     3.826571    -2.938508      12.86
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 O      -4.057850     5.100037    -3.626881     153.52
 H      -3.359575     5.830512    -3.401295      28.63
 C      -4.097539     2.661529    -3.617595      52.07
 H      -4.262469     2.828912    -4.651368      20.56
 C      -3.708484     1.245333    -1.621531      16.23
 C      -3.859331    -0.175252    -0.912383     105.26
 H      -4.391176    -0.639813    -1.635627      24.71
 O      -4.630526    -0.218007     0.282779     232.18
 H      -4.099461     0.008859     1.006271      27.80
 C      -2.520475    -1.006513    -0.750028      76.55
 H      -1.881451    -0.978615    -1.745237      22.51
 C      -2.972965    -2.652078    -0.479936      85.95
 O      -4.142340    -3.196463    -1.436383     221.36
 H      -3.545139    -3.459164    -2.183423      26.46
 H      -3.466480    -2.526573     0.665276      23.45
 H      -2.174992    -3.211124    -0.504371      26.42
 C       1.715677    -1.147290    -0.946428      46.31
 H       2.452118    -1.545773    -1.638257      20.64
 C       1.667985     0.504215     1.011987      74.69
 H       2.250234     1.030998     1.707214      22.62
 C       0.334074     0.247466     1.156018       0.74
 O      -0.470165     0.786338     2.124341     197.44
 C      -0.051922     2.121475     2.764578     105.39
 H       0.529560     2.530378     1.995674      26.65
 H      -0.961740     2.603460     3.010574      25.31
 H       0.489321     1.852109     3.488649      27.88
 C      -0.441594    -0.614472     0.116209      22.03
 O      -1.785181    -0.701814     0.364634     218.93
 C       0.273991    -1.377390    -0.690100      74.27
 H       0.048382    -2.199920    -1.453541      20.99
 C       2.331279    -0.241820    -0.005221       4.32
 C       3.945474     0.145675    -0.228858      39.94
 H       4.115597    -0.206009    -1.376105      20.25
 O       4.130668     1.593368    -0.225758     231.25
 H       5.138365     1.831381    -0.365573      22.16
 C       4.973394    -0.506443     1.110550      72.52
 H       5.036429    -0.119743     2.287018      21.00
 O       4.794284    -1.918285     1.010386     259.75
 H       5.154524    -2.164800     1.914113      27.67
 C       6.358366    -0.205871     0.507239      91.78
 O       6.786724     1.290554     0.497515     264.30
 H       7.162708     1.578187     1.331390      29.71
 H       6.740184    -0.732693    -0.395120      27.55
 H       7.116150    -0.570826     1.413515      25.36
55
name= lig-ACN-Water-frame_848
 C      -3.981310     1.237818    -3.058351      39.96
 H      -4.331513     0.350999    -3.573393      22.35
 C      -3.493510     2.480314    -0.899926      59.12
 H      -3.376871     2.526627     0.202112      19.49
 C      -3.529493     3.679012    -1.564061      11.46
 O      -3.265963     4.921745    -0.906484     214.45
 C      -3.758996     4.807283     0.647657      96.29
 H      -3.241173     5.852846     0.840596      23.63
 H      -2.780751     4.164398     0.984938      19.57
 H      -4.742789     4.834563     0.564054      28.33
 C      -3.866782     3.856750    -2.915280       6.32
 O      -4.036880     5.044461    -3.612069     159.15
 H      -3.509466     5.683389    -2.939747      21.23
 C      -4.214486     2.541472    -3.610554       5.24
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 H      -4.783906     2.521254    -4.517233      24.80
 C      -3.806715     1.203565    -1.613353       4.95
 C      -3.857660    -0.189452    -0.988282      99.41
 H      -4.460747    -0.851746    -1.570394      22.96
 O      -4.701532    -0.187281     0.275767     203.97
 H      -4.142776     0.108210     1.056026      24.35
 C      -2.649016    -1.151564    -0.875196      69.60
 H      -2.064794    -1.014444    -1.926256      20.79
 C      -2.937960    -2.579723    -0.596446     116.80
 O      -4.057219    -3.110060    -1.354843     320.73
 H      -3.898218    -3.240319    -2.207085      34.12
 H      -3.271387    -2.752810     0.565881      23.76
 H      -2.100598    -3.160623    -0.704726      26.72
 C       1.784870    -1.150994    -0.827050      44.51
 H       2.082365    -1.414343    -1.798272      23.57
 C       1.678807     0.389148     0.934515      54.29
 H       2.047492     1.316716     1.331178      20.27
 C       0.224206     0.184597     1.147528      12.12
 O      -0.566303     0.797178     2.138599     213.50
 C      -0.059141     2.096986     2.715992     135.69
 H       0.431671     2.785072     2.174045      29.32
 H      -0.867861     2.607233     3.092845      28.09
 H       0.454841     1.913033     3.517634      29.28
 C      -0.379579    -0.574515     0.231569       7.85
 O      -1.770489    -0.620877     0.267624     141.86
 C       0.340903    -1.373128    -0.805575      54.07
 H      -0.416444    -1.882003    -1.350345      17.34
 C       2.547953    -0.287291    -0.009291      29.31
 C       3.981987     0.088987    -0.208170      96.74
 H       4.502115    -0.383129    -1.186416      22.06
 O       4.124986     1.543706    -0.172345     232.83
 H       5.077225     1.752454     0.126070      22.87
 C       4.906142    -0.330840     0.923478      78.34
 H       4.250260     0.220436     1.864256      21.36
 O       4.848486    -1.963710     1.109498     246.17
 H       5.212079    -2.321009     1.875058      31.71
 C       6.465515    -0.123872     0.722161      75.35
 O       6.758369     1.306842     0.550772     292.45
 H       7.419549     1.420857     1.225033      29.00
 H       6.456690    -0.538440    -0.319037      27.69
 H       7.195480    -0.793441     1.477534      24.61
55
name= lig-ACN-Water-frame_849
 C      -4.153357     1.266282    -2.921580      54.61
 H      -4.424898     0.364785    -3.459391      24.34
 C      -3.532849     2.327361    -0.924619      20.89
 H      -3.258549     2.143188     0.200643      15.48
 C      -3.469695     3.690762    -1.591428     -22.49
 O      -3.280962     4.959064    -0.859986     234.25
 C      -3.723583     4.908729     0.499651      92.34
 H      -3.791414     5.887163     1.205300      24.24
 H      -3.244303     3.970054     1.196400      22.42
 H      -4.497124     4.225193     0.657344      27.84
 C      -3.865447     3.624640    -3.003895       3.29
 O      -3.980404     4.969160    -3.536546     127.23
 H      -3.793165     5.735490    -2.913045      25.69
 C      -4.288660     2.520923    -3.648820      83.06
 H      -4.731754     2.660566    -4.665728      24.72
 C      -3.759603     1.190590    -1.628133      37.59
 C      -4.008814    -0.258285    -0.976637      91.78
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 H      -4.731293    -0.673260    -1.706951      23.54
 O      -4.699097    -0.139525     0.238133     211.80
 H      -4.122067     0.264309     1.045071      21.72
 C      -2.689548    -1.086494    -0.953938      65.92
 H      -2.096958    -0.991082    -2.010955      21.43
 C      -2.889365    -2.616586    -0.668442     111.18
 O      -4.043037    -3.055969    -1.283635     317.75
 H      -3.725752    -3.139808    -2.253566      28.97
 H      -3.024675    -2.644426     0.511185      24.38
 H      -2.019763    -3.108608    -1.005333      24.23
 C       1.819624    -1.205709    -0.899031      44.92
 H       2.378666    -1.860666    -1.476980      22.88
 C       1.686608     0.383739     0.953547      59.57
 H       2.189492     1.167223     1.592790      20.32
 C       0.330308     0.198075     1.153602       0.99
 O      -0.596960     0.872127     2.097843     197.89
 C      -0.097791     2.046772     2.751920     131.88
 H       0.221464     2.485571     1.910297      28.12
 H      -0.988365     2.402704     3.067778      26.20
 H       0.650730     1.941357     3.378776      28.85
 C      -0.406141    -0.720685     0.193820      14.70
 O      -1.810482    -0.551345     0.158074     146.66
 C       0.436942    -1.208979    -0.770358      77.99
 H       0.211302    -1.720882    -1.563561      24.37
 C       2.497132    -0.313842    -0.015799      18.85
 C       4.017814     0.029872    -0.217415      79.97
 H       4.308115    -0.383027    -1.256064      22.33
 O       4.119599     1.528126    -0.153182     251.34
 H       4.787018     1.874194     0.498779      22.55
 C       4.910292    -0.450657     0.961205      84.88
 H       4.556749     0.142077     2.061543      20.94
 O       4.868006    -1.873188     1.148885     235.94
 H       5.271432    -1.754607     2.082766      26.36
 C       6.406346    -0.044435     0.784303      85.81
 O       6.806455     1.311739     0.646630     263.87
 H       7.436999     1.761748     1.343857      27.50
 H       6.929959    -0.615389    -0.065113      26.88
 H       7.058238    -0.492578     1.778268      25.24
55
name= lig-ACN-Water-frame_850
 C      -4.378411     1.305482    -3.009454      41.10
 H      -4.678401     0.378521    -3.535614      26.73
 C      -3.460131     2.364417    -0.893392      34.88
 H      -3.201415     2.386656     0.276402      17.65
 C      -3.458347     3.543991    -1.510924      27.36
 O      -3.313754     4.877469    -0.925975     224.65
 C      -3.732900     4.807259     0.470991      98.18
 H      -4.164651     5.989100     0.505986      23.21
 H      -2.688517     4.706631     1.181088      21.27
 H      -4.662958     4.417236     0.432272      28.36
 C      -3.868308     3.696598    -2.879062       6.05
 O      -3.949885     4.843726    -3.521843     174.75
 H      -3.558987     5.442387    -2.878515      25.00
 C      -4.322772     2.488341    -3.661633      47.24
 H      -4.466242     2.472157    -4.819046      20.76
 C      -3.792754     1.094709    -1.640890      -2.45
 C      -4.058203    -0.207678    -1.009492      87.53
 H      -4.761887    -0.945903    -1.621532      21.76
 O      -4.717245    -0.102415     0.270889     208.41
 H      -4.031749     0.141607     0.983455      23.82
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 C      -2.634081    -1.026793    -0.960014      76.54
 H      -2.191015    -0.743814    -2.040949      23.22
 C      -2.748140    -2.564430    -0.662359      98.14
 O      -4.120369    -3.085096    -1.301887     182.53
 H      -3.938647    -3.557862    -2.321072      24.73
 H      -2.813938    -2.781624     0.454271      26.19
 H      -1.884677    -3.215982    -0.966484      23.70
 C       1.936254    -1.213012    -0.881198      39.48
 H       2.548113    -1.822631    -1.494630      22.44
 C       1.722894     0.430944     1.037279      63.29
 H       2.396856     0.828063     1.890639      19.25
 C       0.265768     0.162254     1.144570       8.57
 O      -0.533250     0.787000     1.980624     199.65
 C      -0.120892     2.070939     2.690659     125.67
 H       0.208340     2.916675     2.214102      28.61
 H      -0.788400     2.462242     3.352730      28.00
 H       0.547874     1.757684     3.344547      28.76
 C      -0.410784    -0.642017     0.162144      -1.86
 O      -1.820241    -0.482937     0.056417     161.03
 C       0.410686    -1.266405    -0.904513      49.48
 H      -0.194822    -1.667505    -1.516905      21.53
 C       2.465482    -0.272193     0.022853      19.62
 C       3.930741     0.058989    -0.134883      97.35
 H       4.281558    -0.137466    -1.155196      22.78
 O       4.121556     1.499487    -0.190504     285.84
 H       4.518194     1.827808     0.684495      21.96
 C       4.976689    -0.430719     1.033572      72.38
 H       4.580218     0.118809     2.124331      19.54
 O       4.900155    -1.828394     1.238422     275.09
 H       5.131139    -2.384495     2.069241      27.08
 C       6.476237    -0.066015     0.866564      76.06
 O       6.848586     1.417446     0.722577     280.74
 H       7.167893     1.427295     1.677116      25.90
 H       7.001490    -0.786271     0.162632      26.64
 H       6.742951    -0.283828     2.055029      23.87
55
name= lig-ACN-Water-frame_851
 C      -4.449430     1.232111    -2.977763      50.03
 H      -4.972723     0.416360    -3.528456      20.27
 C      -3.384698     2.208840    -0.896474      33.98
 H      -3.149351     2.053331     0.253634      18.90
 C      -3.514436     3.519793    -1.552686      10.89
 O      -3.294611     4.683503    -1.018503     202.40
 C      -3.815114     4.904417     0.409588      88.77
 H      -4.129996     6.093332     0.470659      23.05
 H      -2.880729     4.790168     1.233292      22.97
 H      -4.175001     4.120510     0.971160      25.98
 C      -3.926133     3.569619    -2.857928      44.29
 O      -3.898459     4.857418    -3.527932     167.01
 H      -3.364335     5.670302    -3.253013      24.46
 C      -4.273446     2.557597    -3.603224      37.86
 H      -4.567740     2.901441    -4.695527      18.02
 C      -4.001548     1.200312    -1.699103       4.06
 C      -3.951780    -0.242807    -0.974844      75.25
 H      -4.688648    -0.957161    -1.665477      21.74
 O      -4.732006    -0.094210     0.321319     197.50
 H      -4.202318     0.079257     1.070752      27.10
 C      -2.642813    -1.040470    -0.970452      75.67
 H      -2.141464    -0.931590    -2.027659      22.88
 C      -2.830154    -2.562514    -0.772540     114.14
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 O      -4.063031    -3.111995    -1.247571     264.87
 H      -3.752142    -3.608011    -2.119894      26.78
 H      -2.867522    -2.668236     0.302377      25.57
 H      -1.921636    -3.134670    -1.273204      21.79
 C       1.763646    -1.173073    -0.841615      51.16
 H       2.320725    -1.393431    -1.758946      19.17
 C       1.659729     0.308198     1.108727      61.66
 H       1.923579     1.121526     1.898737      18.55
 C       0.337752     0.166509     1.022144      12.99
 O      -0.575364     0.838244     1.969659     185.54
 C      -0.079851     2.014642     2.709927     124.64
 H       0.096752     2.729203     1.992274      28.13
 H      -1.019410     1.996929     3.141027      24.51
 H       0.775923     1.871812     3.254313      27.10
 C      -0.289156    -0.517543    -0.054488      10.59
 O      -1.733255    -0.366270     0.053514     119.91
 C       0.392064    -1.345359    -0.934442      77.07
 H       0.112241    -1.933438    -1.662859      23.00
 C       2.488872    -0.241065     0.118499      21.11
 C       3.995275     0.064992    -0.015210      99.11
 H       4.267419    -0.619736    -0.750909      23.75
 O       4.127327     1.524092    -0.198043     267.03
 H       4.503995     1.918732     0.668795      22.42
 C       4.970520    -0.287031     1.104415      72.15
 H       4.515745     0.375702     2.079560      21.17
 O       4.893957    -1.936841     1.266653     243.02
 H       5.148811    -1.987978     2.173365      29.72
 C       6.557991    -0.010876     1.044043      83.70
 O       6.844005     1.407040     0.810874     315.52
 H       7.445339     1.824650     1.419192      30.01
 H       6.923875    -0.457035     0.063710      27.21
 H       7.260468    -0.523914     1.894743      25.81
55
name= lig-ACN-Water-frame_852
 C      -4.477435     1.288577    -3.006647      51.17
 H      -4.844972     0.367416    -3.511868      23.93
 C      -3.444182     2.124285    -1.019462      56.95
 H      -2.886732     1.916140    -0.075162      18.89
 C      -3.556453     3.380528    -1.511657       2.21
 O      -3.269166     4.654134    -0.898810     239.31
 C      -3.713684     4.992728     0.373478     100.76
 H      -4.697781     5.784774     0.413628      21.10
 H      -2.708783     5.380073     0.939763      22.09
 H      -4.421400     4.191192     0.543062      25.57
 C      -3.874193     3.657692    -2.938767     -10.81
 O      -3.873681     4.872449    -3.580078     144.48
 H      -3.289657     5.344365    -2.840923      20.73
 C      -4.357949     2.466624    -3.675236      46.70
 H      -4.851277     2.576122    -4.734705      20.51
 C      -4.079471     1.039280    -1.592835      28.73
 C      -4.010347    -0.210235    -0.929696      97.57
 H      -4.731243    -0.987048    -1.621366      20.85
 O      -4.701019    -0.143096     0.320246     244.08
 H      -4.075057     0.162084     1.009811      25.46
 C      -2.615839    -0.944601    -0.981795      73.60
 H      -2.205511    -0.727766    -2.006775      22.06
 C      -2.837086    -2.555773    -0.735734     114.23
 O      -4.033860    -3.173185    -1.232670     324.05
 H      -3.956030    -3.355185    -2.093785      35.24
 H      -2.707221    -2.828608     0.254261      27.12
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 H      -1.879594    -3.093040    -1.292555      20.66
 C       1.834483    -0.992572    -0.839689      55.79
 H       2.500271    -1.542298    -1.599523      21.09
 C       1.680889     0.260944     1.179712      60.91
 H       2.269093     1.020275     1.808496      15.78
 C       0.245132     0.262377     0.963775       0.96
 O      -0.568353     0.794164     1.896579     220.03
 C      -0.120803     1.952811     2.690838     124.79
 H       0.067428     2.801605     2.106069      26.50
 H      -0.671209     2.497341     3.438467      24.97
 H       0.729572     1.790360     3.293500      25.46
 C      -0.412116    -0.452260    -0.163104      15.88
 O      -1.684532    -0.337435    -0.018873     194.17
 C       0.428860    -1.325842    -0.915828      67.63
 H      -0.029037    -1.931828    -1.727206      19.10
 C       2.472341    -0.378521     0.178910      35.12
 C       4.075633     0.011553     0.037328      65.61
 H       4.510887    -0.160818    -0.868571      19.23
 O       4.160644     1.528959    -0.208500     277.72
 H       4.882862     1.951467     0.340194      20.78
 C       5.017129    -0.350873     1.308333      84.91
 H       4.651035    -0.168248     2.488164      18.01
 O       4.884724    -1.828741     1.326540     262.48
 H       5.174429    -2.125118     2.275699      28.25
 C       6.548221     0.047642     1.019797      72.51
 O       6.827176     1.426763     0.888520     361.66
 H       7.434335     1.516243     1.615807      28.32
 H       6.783851    -0.594227     0.108673      28.34
 H       7.107088    -0.413411     1.968618      24.75
55
name= lig-ACN-Water-frame_853
 C      -4.529689     1.190651    -2.975002      64.77
 H      -4.903718     0.393526    -3.603022      21.22
 C      -3.497684     2.156444    -0.991799      12.77
 H      -2.995692     2.133419    -0.066806      19.53
 C      -3.592908     3.502657    -1.643420     -21.74
 O      -3.123377     4.624309    -0.918777     177.25
 C      -3.780496     5.024311     0.412207      93.08
 H      -4.430219     5.917193    -0.068156      20.99
 H      -3.090770     5.603922     1.179127      24.14
 H      -3.863132     4.304668     1.292924      22.29
 C      -3.916141     3.568528    -3.026623      16.99
 O      -3.790808     4.876052    -3.553557     175.34
 H      -3.799625     5.659108    -2.986523      22.52
 C      -4.457825     2.471532    -3.693739      64.41
 H      -4.642752     2.403965    -4.793197      28.47
 C      -4.052085     1.012277    -1.733063      18.62
 C      -4.138731    -0.369486    -0.931198      85.66
 H      -4.841804    -1.286895    -1.467963      18.71
 O      -4.651014    -0.214690     0.383876     251.83
 H      -3.948860     0.120840     1.125353      20.03
 C      -2.707842    -0.956372    -1.003668      87.14
 H      -2.386607    -0.773638    -2.039606      22.11
 C      -2.695258    -2.513858    -0.690848      95.43
 O      -4.050368    -3.208874    -1.236184     260.67
 H      -3.897282    -3.155870    -2.203577      30.24
 H      -2.764441    -2.662918     0.280801      27.26
 H      -1.739242    -3.148220    -1.210747      19.74
 C       1.956474    -1.050705    -0.941083      33.15
 H       2.656471    -1.718481    -1.623503      18.07
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 C       1.699095     0.265347     1.135494      57.36
 H       2.029176     0.558111     2.158166      16.63
 C       0.320250     0.327860     0.944987      13.19
 O      -0.663166     0.812708     1.907035     203.19
 C      -0.086903     1.990110     2.680050     100.93
 H       0.297002     2.715138     2.000793      24.81
 H      -1.035239     1.921764     3.252889      21.17
 H       0.724679     1.429431     3.129522      22.90
 C      -0.305578    -0.410541    -0.040289      -5.98
 O      -1.858269    -0.331941    -0.101635     149.43
 C       0.503220    -1.133192    -0.952805      49.73
 H      -0.062492    -1.878189    -1.699638      17.63
 C       2.624953    -0.352660     0.227494      23.64
 C       4.072269     0.070508     0.179704      83.61
 H       4.385168    -0.701641    -0.448380      24.10
 O       4.204551     1.490830    -0.181682     274.70
 H       5.139594     1.720791     0.089881      17.31
 C       5.018356    -0.419955     1.399578      83.22
 H       4.676095     0.443682     2.213810      19.59
 O       4.905793    -1.770578     1.422043     285.24
 H       5.242685    -2.555507     2.058846      26.08
 C       6.436862    -0.053563     1.032843     109.20
 O       6.791095     1.457402     0.903401     315.17
 H       7.279470     1.817128     1.627813      32.62
 H       6.888062    -0.525420     0.119625      29.96
 H       7.121017    -0.378270     1.895072      27.14
55
name= lig-ACN-Water-frame_854
 C      -4.586445     1.138567    -3.109044      38.83
 H      -5.030251     0.273211    -3.526641      25.14
 C      -3.628808     2.226909    -1.049098      71.32
 H      -3.532141     2.184434    -0.025935      21.89
 C      -3.550094     3.487805    -1.635395       8.49
 O      -2.970057     4.564467    -0.960724     151.32
 C      -3.782325     5.142206     0.420648      45.91
 H      -4.956174     5.524051     0.501224      23.24
 H      -2.933393     5.800151     0.481640      23.15
 H      -4.044266     4.071127     0.924568      21.87
 C      -3.993951     3.623258    -2.970604     -12.28
 O      -3.746948     4.855840    -3.634670     114.05
 H      -3.869657     5.394692    -2.856205      27.27
 C      -4.492342     2.434619    -3.701121      46.38
 H      -4.705013     2.696708    -4.713369      19.10
 C      -4.020928     1.062167    -1.676840     -57.20
 C      -4.160521    -0.433528    -0.936477      55.85
 H      -5.115336    -0.996807    -1.560402      20.20
 O      -4.639872    -0.286991     0.465323     190.79
 H      -3.805495    -0.191914     1.128462      20.39
 C      -2.785201    -1.170545    -1.127622      63.34
 H      -2.500417    -1.019131    -2.118224      24.02
 C      -2.788887    -2.558387    -0.696749     115.69
 O      -3.910838    -3.161687    -1.220112     271.15
 H      -3.753419    -3.539036    -2.270096      25.98
 H      -2.765265    -2.596220     0.280708      27.77
 H      -1.675003    -3.118256    -0.997136      20.54
 C       2.031075    -1.078594    -0.829733      52.61
 H       2.559296    -1.474329    -1.793383      19.99
 C       1.720035     0.276086     1.150541      43.66
 H       2.187937     0.637768     2.053594      18.33
 C       0.268003     0.307197     1.035165       0.83
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 O      -0.629485     0.890406     1.854005     223.40
 C      -0.113506     1.874632     2.727167     125.14
 H       0.124084     2.789909     2.126453      25.26
 H      -0.805233     2.557964     3.380083      24.08
 H       0.662748     1.893759     3.539934      24.70
 C      -0.367647    -0.424805    -0.100969       0.28
 O      -1.794559    -0.260836    -0.078416      79.62
 C       0.628347    -0.958250    -1.014599      48.97
 H       0.243591    -1.689942    -1.962563      19.93
 C       2.568780    -0.262555     0.134971      29.83
 C       4.119348    -0.037502     0.238005      78.92
 H       4.651997    -0.423520    -0.591998      18.10
 O       4.256090     1.375505    -0.134389     269.63
 H       5.178216     1.783868     0.000430      21.12
 C       4.977584    -0.211553     1.419798      93.92
 H       4.704696    -0.124463     2.615803      19.88
 O       4.872170    -1.896119     1.512383     229.08
 H       5.436821    -1.732474     2.250167      29.84
 C       6.523829    -0.031062     1.105529      79.96
 O       6.676728     1.388193     0.847350     312.26
 H       7.396274     1.642821     1.518735      28.07
 H       6.543984    -0.503782     0.111150      31.43
 H       7.168660    -0.582884     1.805317      29.11
55
name= lig-ACN-Water-frame_855
 C      -4.498390     1.201889    -3.051232      74.00
 H      -4.814050     0.423124    -3.689743      27.75
 C      -3.774153     2.192852    -0.976851      12.98
 H      -3.512835     2.047786     0.076294      18.61
 C      -3.541596     3.466126    -1.625497       6.88
 O      -2.963873     4.590264    -0.952443     211.89
 C      -3.690621     5.113240     0.278614      67.93
 H      -4.751302     5.425356    -0.223699      23.46
 H      -3.349874     5.949129     0.824592      26.14
 H      -3.353389     4.360223     1.254630      20.89
 C      -3.999902     3.616679    -2.985219       8.99
 O      -3.790177     4.792676    -3.691078     160.66
 H      -3.279702     5.554706    -3.238197      25.24
 C      -4.492308     2.479561    -3.695975      70.14
 H      -5.043151     2.527807    -4.578207      16.30
 C      -4.186899     0.979127    -1.738413      13.78
 C      -4.119951    -0.251771    -0.925007      84.99
 H      -4.984075    -1.000767    -1.511219      20.66
 O      -4.625583    -0.386375     0.426624     190.87
 H      -3.980904    -0.162008     1.147711      22.90
 C      -2.793225    -1.119651    -1.129697      56.91
 H      -2.425717    -1.020809    -2.064098      25.16
 C      -2.757720    -2.653842    -0.568760     107.63
 O      -3.880700    -3.238753    -1.290372     268.12
 H      -3.453326    -3.759428    -2.146051      26.28
 H      -2.974750    -2.753369     0.404512      24.51
 H      -1.679718    -3.242077    -0.942211      18.41
 C       1.986803    -0.954703    -0.814396      24.06
 H       2.766786    -1.397093    -1.505996      18.05
 C       1.688159     0.334454     1.178434      97.88
 H       2.069205     1.141547     1.760420      19.40
 C       0.296014     0.179361     1.021004       5.20
 O      -0.583752     0.948371     1.883615     200.04
 C      -0.128377     2.038465     2.834953      61.48
 H       0.579458     2.642626     2.207920      23.63
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 H      -1.247909     2.214178     3.241435      21.03
 H       0.532399     1.238001     3.382076      21.53
 C      -0.323957    -0.388295    -0.164640      21.09
 O      -1.697845    -0.299544    -0.193131     143.11
 C       0.559925    -0.937402    -1.079454      65.39
 H       0.145342    -1.234165    -2.244641      19.00
 C       2.584637    -0.251343     0.225169      58.18
 C       4.140602    -0.024209     0.146054      58.73
 H       4.505168    -0.815113    -0.538345      21.98
 O       4.235607     1.386192    -0.142465     276.08
 H       5.141416     1.641954     0.251689      19.01
 C       4.977501    -0.419400     1.511628      80.38
 H       4.404166     0.330029     2.344427      22.00
 O       4.908318    -1.863495     1.674241     320.54
 H       5.242560    -2.400388     2.370568      31.63
 C       6.444008    -0.051629     1.090405     125.24
 O       6.693624     1.334500     0.845184     271.26
 H       7.274697     1.803119     1.637238      27.62
 H       6.760837    -0.692353     0.272777      32.26
 H       7.166661    -0.197056     1.841099      27.93
55
name= lig-ACN-Water-frame_856
 C      -4.463435     1.223622    -3.063340      24.80
 H      -4.652124     0.347544    -3.668672      20.02
 C      -3.863712     2.182836    -0.916735      52.17
 H      -3.394675     2.071562     0.153998      16.96
 C      -3.605493     3.431443    -1.579291      -7.28
 O      -2.932931     4.616661    -0.981735     208.84
 C      -3.589479     5.064374     0.140483     107.24
 H      -4.882896     4.976538     0.017125      24.86
 H      -3.247980     6.052178     0.062034      23.62
 H      -3.733771     4.324894     1.155534      22.05
 C      -3.912604     3.587245    -2.971976      -1.29
 O      -3.853925     4.764841    -3.771974     175.92
 H      -3.150479     5.258161    -3.255701      23.87
 C      -4.512203     2.535993    -3.634476      52.99
 H      -4.743661     2.678262    -4.681468      28.44
 C      -4.256567     1.130300    -1.613367      19.29
 C      -4.079499    -0.369898    -0.970096      76.10
 H      -4.661578    -1.256664    -1.665993      21.42
 O      -4.628318    -0.425733     0.363742     215.25
 H      -4.125938     0.076627     0.964969      26.31
 C      -2.622480    -1.015186    -0.957305      99.88
 H      -2.563169    -1.149512    -1.995122      24.09
 C      -2.781171    -2.606150    -0.535066      83.23
 O      -3.883081    -3.393908    -1.353932     260.95
 H      -3.584848    -3.584274    -2.249055      29.44
 H      -2.976503    -2.652166     0.519497      25.39
 H      -1.620170    -3.121911    -0.606486      20.87
 C       1.920653    -0.839087    -0.902112      46.60
 H       2.475509    -1.411220    -1.628212      22.19
 C       1.691513     0.447639     1.162212      63.44
 H       1.944689     1.126288     1.982929      19.77
 C       0.311588     0.242306     1.060806       9.14
 O      -0.595013     0.943564     1.834324     178.94
 C      -0.076787     1.956732     2.873254      97.47
 H       0.420987     3.029141     2.660450      22.43
 H      -1.060324     2.572085     3.263834      22.74
 H       0.344440     1.732075     3.985100      23.38
 C      -0.277257    -0.388864    -0.151509      11.84
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 O      -1.680564    -0.335712    -0.337412     227.45
 C       0.563047    -0.930555    -1.131641      45.16
 H       0.090222    -1.370756    -2.209249      20.23
 C       2.576719    -0.304126     0.337452      33.32
 C       4.030940    -0.103125     0.190800      72.82
 H       4.386533    -0.477374    -0.820094      20.73
 O       4.247518     1.402917    -0.168306     227.31
 H       5.008578     1.861331     0.299842      18.24
 C       4.972668    -0.529148     1.434214      85.06
 H       4.691609     0.150501     2.462481      20.43
 O       4.901452    -1.873497     1.807502     259.68
 H       5.202517    -2.196996     2.813560      25.92
 C       6.457208    -0.169555     1.223264     101.24
 O       6.713280     1.340792     0.865436     291.24
 H       7.034432     1.693562     1.782493      28.03
 H       6.845002    -0.620663     0.337611      29.85
 H       6.909189    -0.532633     2.063849      30.37
55
name= lig-ACN-Water-frame_857
 C      -4.524873     1.230110    -2.981326      62.29
 H      -4.769264     0.300269    -3.548534      23.14
 C      -3.818931     2.325312    -0.820962       0.59
 H      -3.668331     2.314122     0.395463      17.85
 C      -3.614819     3.499209    -1.574925      16.15
 O      -2.893418     4.476950    -1.127442     241.64
 C      -3.652816     5.119510     0.120520      71.67
 H      -4.911370     5.153572    -0.019435      24.62
 H      -3.409958     6.109693     0.358090      25.89
 H      -2.887328     4.688572     0.981645      20.26
 C      -3.923409     3.587729    -2.950119      -9.05
 O      -3.842029     4.736347    -3.756932     191.36
 H      -3.526983     5.536215    -3.377327      25.48
 C      -4.472007     2.449834    -3.646630      47.71
 H      -4.481799     2.621359    -4.762454      25.88
 C      -4.232513     1.021672    -1.613244     -28.50
 C      -4.013759    -0.427342    -0.989781      86.50
 H      -4.756897    -1.133812    -1.686441      22.38
 O      -4.685297    -0.449406     0.293477     174.34
 H      -4.015417    -0.125423     1.013038      23.10
 C      -2.619420    -1.163654    -1.071849      80.01
 H      -2.122362    -1.102479    -1.980757      23.88
 C      -2.878200    -2.561977    -0.573629     111.72
 O      -3.767834    -3.430647    -1.274976     288.93
 H      -3.640917    -3.399540    -2.148329      33.51
 H      -3.352429    -2.633210     0.460358      23.29
 H      -1.806817    -3.187350    -0.658367      21.19
 C       1.995683    -0.835452    -0.921570      60.05
 H       2.671248    -1.028266    -1.668094      23.24
 C       1.694388     0.451225     1.189018      82.46
 H       2.358561     0.758892     2.033609      19.07
 C       0.270077     0.392555     0.987830       0.02
 O      -0.594988     1.009312     1.892351     177.85
 C      -0.154077     1.954875     2.936332      42.55
 H       0.755271     2.304905     2.192539      19.79
 H      -1.187162     2.476606     3.118876      21.41
 H       0.465945     1.242897     3.753991      21.88
 C      -0.297968    -0.413135    -0.114212      18.78
 O      -1.612525    -0.202732    -0.284128     163.77
 C       0.563842    -0.886836    -1.096054      64.88
 H       0.165141    -1.675262    -1.902377      20.50
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 C       2.436476    -0.299514     0.209568      28.03
 C       4.040415    -0.099016     0.242747      74.15
 H       4.510498    -0.826846    -0.593285      22.03
 O       4.212531     1.385131    -0.158002     211.06
 H       5.049733     1.548586     0.351908      20.38
 C       4.968796    -0.391750     1.376616      82.98
 H       4.418835     0.101631     2.342402      20.86
 O       4.856010    -2.017755     1.911320     190.25
 H       5.203700    -1.553103     2.736617      25.63
 C       6.533554    -0.200339     1.262572     105.05
 O       6.700909     1.203329     1.029303     343.47
 H       7.180688     1.691504     1.667087      31.37
 H       6.884839    -0.847394     0.480699      29.32
 H       7.033019    -0.376407     2.096511      30.63
55
name= lig-ACN-Water-frame_858
 C      -4.574255     1.160754    -2.867486      32.30
 H      -4.962461     0.299610    -3.501417      24.39
 C      -3.847451     2.199055    -0.892135      51.49
 H      -3.654248     2.305452     0.308621      17.19
 C      -3.647367     3.413646    -1.668930     -20.31
 O      -2.888266     4.608276    -1.092975     198.58
 C      -3.499683     5.219731     0.101454     100.30
 H      -4.660757     4.670448     0.071273      24.01
 H      -3.535106     6.251619    -0.088571      24.48
 H      -3.337194     4.657650     1.179864      22.53
 C      -4.046039     3.540610    -3.036445      26.87
 O      -3.805881     4.731314    -3.730967     158.16
 H      -3.812037     5.383815    -2.953240      26.06
 C      -4.349047     2.373919    -3.659580      48.76
 H      -4.804563     2.211068    -4.707217      18.84
 C      -4.068372     1.078702    -1.531195      35.63
 C      -4.048330    -0.345759    -1.075081      88.13
 H      -4.761099    -1.035733    -1.761702      24.17
 O      -4.678072    -0.479103     0.265642     152.61
 H      -3.969106    -0.384777     1.050494      22.41
 C      -2.671461    -1.141731    -1.195638      49.55
 H      -2.352338    -1.229757    -2.236440      22.87
 C      -2.795675    -2.628320    -0.518520      97.11
 O      -3.741026    -3.435839    -1.222915     288.00
 H      -3.401042    -3.648961    -2.185610      27.98
 H      -3.215101    -2.260492     0.522720      21.88
 H      -1.720592    -3.058835    -0.212612      22.65
 C       1.978048    -0.872240    -1.016605      28.87
 H       2.576064    -1.222481    -1.784743      22.28
 C       1.666518     0.303546     1.160692      65.46
 H       1.912291     0.846964     2.146826      17.43
 C       0.295430     0.511252     0.999197      15.20
 O      -0.677725     1.009754     1.882305     223.25
 C      -0.088146     1.866144     2.859667     111.03
 H       0.769975     2.809149     2.856072      20.76
 H      -0.788438     2.617749     3.384655      23.20
 H       0.086747     1.179971     3.875857      22.15
 C      -0.262089    -0.278557    -0.056324      -8.71
 O      -1.718277    -0.145059    -0.182270      59.21
 C       0.587461    -0.967883    -1.057184      51.25
 H       0.054777    -1.436543    -1.925884      21.38
 C       2.594443    -0.155969     0.190485      24.74
 C       4.042182    -0.094361     0.154058      84.61
 H       4.339986    -0.826070    -0.757594      20.68
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 O       4.205721     1.302698    -0.105765     238.43
 H       5.066091     1.800858    -0.013618      24.40
 C       4.904479    -0.482245     1.545399      61.88
 H       4.771126     0.414999     2.267888      21.82
 O       4.811532    -1.916149     1.949524     323.36
 H       5.064111    -2.424894     2.680568      30.93
 C       6.487253    -0.249734     1.329183     113.01
 O       6.748986     1.155807     1.129593     345.15
 H       7.274817     1.463635     1.921861      27.36
 H       6.975314    -0.758389     0.511626      28.28
 H       6.847182    -0.635366     2.173886      29.60
55
name= lig-ACN-Water-frame_859
 C      -4.502737     1.124418    -2.914863      62.56
 H      -4.971121     0.148951    -3.227300      23.52
 C      -3.734027     2.282638    -0.900327      32.06
 H      -3.253554     2.121040     0.160750      17.06
 C      -3.598928     3.473314    -1.641923       6.07
 O      -2.963823     4.635659    -1.109534     249.93
 C      -3.505144     5.215589     0.074188      97.70
 H      -4.767334     5.125051     0.203120      23.53
 H      -3.374229     6.321401     0.022258      25.22
 H      -2.682152     5.158211     1.015835      23.11
 C      -4.000007     3.489107    -3.043959      -7.23
 O      -3.817171     4.741074    -3.682663     151.23
 H      -3.451347     5.422507    -2.983750      23.28
 C      -4.428476     2.203981    -3.696411      63.23
 H      -4.812203     2.367287    -4.752253      19.19
 C      -4.062075     1.003786    -1.615786      15.72
 C      -4.086867    -0.395220    -1.037071      96.62
 H      -4.810487    -0.950791    -1.746618      23.69
 O      -4.611503    -0.487769     0.246417     235.00
 H      -3.940014    -0.185056     0.863648      26.51
 C      -2.679568    -1.058305    -1.100498      76.80
 H      -2.305921    -0.935234    -2.150813      22.85
 C      -2.684895    -2.486262    -0.458760      91.91
 O      -3.716750    -3.459546    -1.168031     183.67
 H      -3.161730    -3.844443    -2.096292      24.76
 H      -3.242478    -2.632114     0.642283      19.93
 H      -1.697618    -3.013202    -0.496672      22.53
 C       1.937910    -0.816153    -0.948519      57.37
 H       2.438665    -1.405829    -1.674795      20.63
 C       1.703601     0.312412     1.186019      64.86
 H       2.362921     0.699066     2.064120      15.85
 C       0.248995     0.398627     0.951881      -1.44
 O      -0.614302     1.072454     1.798897     137.24
 C      -0.077954     1.876523     3.043861      56.89
 H       0.915908     2.289595     2.326809      18.84
 H      -1.032687     2.386556     3.091667      21.76
 H       0.397851     1.187802     3.949813      22.02
 C      -0.368282    -0.183199    -0.205853      14.06
 O      -1.796330    -0.230084    -0.183586     166.40
 C       0.483244    -0.942502    -0.964641      65.35
 H       0.072160    -1.354793    -1.817788      23.56
 C       2.525355    -0.243480     0.094297      26.11
 C       4.144137    -0.132390     0.230998      49.00
 H       4.847962    -0.587744    -0.634020      17.52
 O       4.252341     1.325489    -0.102216     243.03
 H       5.221333     1.299316     0.076041      19.67
 C       4.961448    -0.536658     1.637212      92.62
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 H       4.460058    -0.048060     2.508941      21.66
 O       4.636497    -1.832523     1.900900     276.29
 H       5.461352    -2.130781     2.447149      26.86
 C       6.398374    -0.339680     1.411392     108.34
 O       6.857459     1.157576     1.219534     367.04
 H       7.033580     1.692860     2.148679      26.98
 H       6.609175    -0.855825     0.460762      30.43
 H       6.954189    -0.697011     2.184109      29.37
55
name= lig-ACN-Water-frame_860
 C      -4.470536     0.991357    -3.032335      26.22
 H      -4.796511     0.143091    -3.672957      20.63
 C      -3.513142     2.202792    -0.954405      58.73
 H      -3.195620     2.315960     0.091725      19.95
 C      -3.579434     3.442783    -1.630940       8.84
 O      -3.075022     4.631069    -1.208992     235.35
 C      -3.472313     5.365709     0.108739      65.06
 H      -4.539744     4.907380     0.642558      23.56
 H      -3.448891     6.478467    -0.148176      22.36
 H      -2.749303     4.784859     0.918013      21.39
 C      -3.878890     3.445523    -3.023133      11.80
 O      -3.863403     4.690406    -3.657344     206.96
 H      -3.162591     5.169010    -3.226505      25.83
 C      -4.494705     2.390866    -3.716917      40.04
 H      -4.711056     2.314031    -4.787405      23.51
 C      -4.095661     1.061054    -1.604982      22.48
 C      -4.049065    -0.418003    -1.014086      95.93
 H      -4.602018    -1.216367    -1.539288      23.35
 O      -4.579163    -0.467796     0.342121     226.45
 H      -4.147238     0.070430     0.986698      25.57
 C      -2.651082    -1.025315    -0.969481      94.01
 H      -2.184796    -1.143911    -2.018400      22.41
 C      -2.702397    -2.496496    -0.545718     107.97
 O      -3.593358    -3.414734    -1.066310     274.50
 H      -3.339227    -3.647908    -2.107090      24.98
 H      -2.663390    -2.350595     0.731602      21.90
 H      -1.687795    -2.794225    -0.690739      24.27
 C       1.785165    -0.892531    -0.948091      31.05
 H       2.447266    -1.303013    -1.761634      20.09
 C       1.707852     0.328909     1.073606      62.26
 H       2.021098     0.707092     2.108240      17.34
 C       0.312888     0.341628     0.985470       5.63
 O      -0.524514     1.119383     1.802520     187.66
 C      -0.075353     1.816884     2.982358      97.10
 H       0.947590     2.710257     2.834724      21.35
 H      -0.690503     2.537954     3.494294      24.24
 H       0.172645     0.965075     3.815356      23.55
 C      -0.493686    -0.184631    -0.215211       5.85
 O      -1.834883    -0.273628    -0.162532     169.88
 C       0.394750    -0.901040    -1.120318      62.07
 H       0.066170    -1.619765    -1.687727      22.43
 C       2.571271    -0.344242     0.242363      22.46
 C       4.138508    -0.087052     0.320899      71.89
 H       4.402685    -1.026266    -0.368588      18.97
 O       4.406082     1.334367    -0.062592     272.01
 H       5.142815     1.847696     0.286752      22.62
 C       4.761763    -0.343027     1.634401      85.26
 H       4.550237     0.395194     2.374300      24.01
 O       4.483138    -1.956397     1.863797     216.33
 H       5.355593    -2.443337     2.289206      26.06
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 C       6.487699    -0.234669     1.466785      94.63
 O       6.901597     1.041006     1.261151     331.33
 H       7.031281     1.502329     2.252871      27.17
 H       6.763743    -0.782117     0.538917      29.11
 H       7.023421    -0.778605     2.249028      28.31
55
name= lig-ACN-Water-frame_861
 C      -4.439427     1.186213    -3.059455      74.59
 H      -4.656296     0.257950    -3.545020      23.14
 C      -3.444268     2.065545    -1.032721      45.94
 H      -3.264393     1.930177    -0.044878      23.52
 C      -3.509012     3.337329    -1.671676      -7.24
 O      -3.176567     4.753817    -1.222101     180.86
 C      -3.397216     5.289447     0.100605      93.40
 H      -4.606646     5.025357     0.311328      21.77
 H      -3.456782     6.497903    -0.125690      21.91
 H      -2.536268     5.312569     0.995849      22.20
 C      -3.910958     3.459006    -3.044510       4.18
 O      -3.876322     4.644144    -3.693708     185.72
 H      -3.320915     5.263490    -3.178001      23.89
 C      -4.446746     2.344609    -3.675230      79.99
 H      -4.728280     2.653989    -4.619787      25.84
 C      -4.066058     0.957222    -1.718985      31.95
 C      -4.012655    -0.339721    -0.941524      98.32
 H      -4.713003    -0.856612    -1.536997      24.34
 O      -4.622268    -0.455151     0.448452     173.33
 H      -4.044449     0.154075     1.096649      22.09
 C      -2.654880    -1.079342    -1.066638      62.12
 H      -2.373409    -0.807872    -2.179120      21.71
 C      -2.477526    -2.527596    -0.511912      97.08
 O      -3.557112    -3.385610    -1.001809     324.13
 H      -3.564758    -3.368195    -1.905385      32.68
 H      -2.785588    -2.656738     0.719546      21.44
 H      -1.565897    -2.951082    -0.737331      23.87
 C       1.837396    -0.949741    -0.913356      31.15
 H       2.370393    -1.472963    -1.804910      20.71
 C       1.625322     0.341914     1.130818      55.37
 H       2.057355     1.003612     1.898478      15.96
 C       0.225997     0.407041     0.909491      17.18
 O      -0.510286     1.186241     1.797499     192.79
 C      -0.004991     1.750963     3.008616      77.76
 H       1.101138     2.528972     2.903412      18.52
 H      -0.992752     2.149800     3.174973      22.14
 H       0.282982     0.939877     3.828790      21.93
 C      -0.358888    -0.317198    -0.105044       8.21
 O      -1.814319    -0.200826    -0.006278      79.56
 C       0.337013    -0.878569    -1.205219      51.83
 H      -0.109421    -1.344353    -1.932125      21.39
 C       2.500972    -0.349157     0.214586      29.57
 C       4.000824    -0.078427     0.303612      76.77
 H       4.710314    -0.486087    -0.545161      17.14
 O       4.496545     1.326012    -0.059649     241.65
 H       5.010220     1.332501     0.777620      18.45
 C       4.800110    -0.410902     1.660897      93.26
 H       4.374679     0.033565     2.456278      24.19
 O       4.356034    -1.905788     1.834494     282.96
 H       4.945882    -2.450685     2.376013      29.95
 C       6.372836    -0.298873     1.488288      88.02
 O       6.975623     1.064337     1.292746     371.80
 H       7.334570     1.616526     2.129264      29.92
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 H       6.740278    -0.922842     0.639185      27.18
 H       6.585351    -0.644153     2.546308      25.69
55
name= lig-ACN-Water-frame_862
 C      -4.474249     1.071003    -3.034613      36.31
 H      -5.048996     0.352431    -3.565812      23.24
 C      -3.475287     2.121395    -1.048035      62.06
 H      -3.051175     2.011650    -0.184151      19.11
 C      -3.393910     3.412707    -1.650292      25.87
 O      -3.218248     4.724043    -1.252047     242.79
 C      -3.407435     5.274519     0.045258      74.26
 H      -4.369011     4.876065     0.817756      23.68
 H      -3.448226     6.475354    -0.105063      22.13
 H      -2.429212     4.847164     0.739985      23.82
 C      -3.941758     3.504933    -2.976311      -1.42
 O      -3.863944     4.679262    -3.760640     134.96
 H      -3.870091     5.446698    -3.060362      25.08
 C      -4.375495     2.402555    -3.770099      48.69
 H      -4.873329     2.322922    -4.641284      21.47
 C      -3.906270     0.935744    -1.727627      25.13
 C      -4.124578    -0.430492    -0.915886      94.30
 H      -4.696988    -1.117145    -1.381311      24.43
 O      -4.634633    -0.381450     0.429828     214.03
 H      -3.964057    -0.099952     1.198396      21.27
 C      -2.590953    -1.017956    -0.953197      64.36
 H      -2.024324    -0.893357    -1.988290      20.87
 C      -2.360892    -2.561895    -0.537068      94.37
 O      -3.551741    -3.373290    -0.958013     300.32
 H      -3.492084    -3.427957    -1.915834      30.82
 H      -2.299618    -2.373838     0.721177      22.42
 H      -1.464338    -2.924995    -0.764012      24.59
 C       1.829161    -0.965024    -0.968534      46.37
 H       2.671118    -1.460823    -1.605594      19.31
 C       1.636978     0.373199     1.133245      72.03
 H       2.202742     0.964816     1.772779      16.55
 C       0.294522     0.474158     0.968834       6.41
 O      -0.588985     1.204078     1.724000     197.86
 C      -0.000901     1.691693     3.100430      69.85
 H       0.891621     2.531860     2.614732      18.13
 H      -0.583956     2.426487     3.675732      23.44
 H       0.442963     0.847503     3.728248      23.10
 C      -0.430556    -0.384898    -0.053508      12.25
 O      -1.734100    -0.211720     0.003934     155.56
 C       0.482384    -0.872383    -1.072745      63.36
 H       0.105722    -1.016784    -2.032235      20.92
 C       2.347657    -0.257090     0.116504      18.67
 C       4.027967    -0.096927     0.220052      43.53
 H       4.235655    -0.956909    -0.597099      20.44
 O       4.481439     1.325070     0.008395     245.99
 H       5.025210     1.855262     0.615243      20.68
 C       4.707119    -0.589033     1.571170     110.85
 H       4.504374     0.086643     2.315980      23.97
 O       4.278597    -1.825841     1.806364     331.55
 H       4.724887    -2.161962     2.561335      29.68
 C       6.254639    -0.365195     1.624627      96.25
 O       6.989668     1.060665     1.267111     301.10
 H       7.139282     1.408335     2.173679      30.19
 H       6.712154    -1.079222     0.877620      27.29
 H       6.897540    -0.686269     2.541532      27.07
55
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name= lig-ACN-Water-frame_863
 C      -4.472709     1.054355    -3.044111      63.52
 H      -5.022269     0.197958    -3.409179      22.99
 C      -3.393584     2.250976    -0.975911      29.73
 H      -3.085257     2.305434    -0.012981      20.57
 C      -3.488313     3.446977    -1.758456       0.35
 O      -3.230208     4.721697    -1.278960     198.91
 C      -3.338331     5.167770     0.124382      73.67
 H      -4.394774     4.626089     0.531450      23.97
 H      -3.411357     6.420618     0.066166      21.36
 H      -2.285591     4.921645     0.748236      22.95
 C      -3.916215     3.485639    -3.133250       1.42
 O      -3.880792     4.752921    -3.771806     175.69
 H      -3.970272     5.471129    -3.103882      27.09
 C      -4.366242     2.273172    -3.679462      63.32
 H      -4.643857     2.575858    -4.617027      22.64
 C      -3.951474     0.940094    -1.715363     -26.37
 C      -3.971702    -0.507921    -0.944560      84.84
 H      -4.527687    -1.118407    -1.518173      25.08
 O      -4.670017    -0.303109     0.370080     210.72
 H      -3.966503     0.074184     0.922685      25.68
 C      -2.508668    -1.061527    -0.826307      92.00
 H      -2.338629    -0.849313    -2.007340      20.99
 C      -2.390576    -2.519829    -0.566688     116.05
 O      -3.475281    -3.333487    -0.886326     249.08
 H      -3.323955    -3.720422    -1.937166      25.70
 H      -2.225374    -2.871174     0.622028      21.73
 H      -1.649031    -2.857945    -1.128111      23.99
 C       1.904859    -0.872547    -0.936793      36.58
 H       2.295613    -1.234566    -1.952625      20.05
 C       1.713188     0.490789     1.087414      63.31
 H       2.095937     0.866784     1.959598      16.32
 C       0.234339     0.422416     1.061455      -2.95
 O      -0.688390     1.252943     1.838148     188.81
 C       0.025949     1.694053     3.027898      97.08
 H       1.078313     2.450529     2.854449      20.97
 H      -0.833259     2.050814     3.677818      23.12
 H       0.448021     0.818627     3.461139      26.31
 C      -0.272420    -0.275053    -0.003808      12.56
 O      -1.751095    -0.248155    -0.039512     182.85
 C       0.436669    -0.920919    -1.022106      49.10
 H      -0.127854    -1.505443    -1.837920      17.92
 C       2.598047    -0.165298     0.113847      26.51
 C       4.013430    -0.097410     0.172356     102.28
 H       4.644353    -0.548894    -0.721920      19.60
 O       4.355468     1.300014    -0.019363     253.32
 H       5.079315     1.247829     0.622622      20.64
 C       4.591415    -0.395908     1.524507      83.27
 H       4.035155     0.213830     2.141532      24.65
 O       4.211532    -1.937345     1.812120     232.48
 H       4.514244    -2.261150     2.786225      28.37
 C       6.372375    -0.383853     1.607418      61.26
 O       6.842870     0.890088     1.253232     369.35
 H       7.138201     1.468834     1.973534      31.75
 H       6.828024    -1.066926     0.829388      25.51
 H       6.324722    -0.657539     2.787615      24.68
55
name= lig-ACN-Water-frame_864
 C      -4.402861     1.048317    -2.894584      33.41
 H      -4.596097     0.138845    -3.538967      21.98
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 C      -3.452988     2.215964    -1.111412      65.39
 H      -3.201117     2.264132    -0.044605      21.06
 C      -3.592587     3.439308    -1.775392      -6.28
 O      -3.205627     4.790039    -1.291074     197.87
 C      -3.267915     4.998073     0.150814      97.33
 H      -4.262579     4.539740     0.757357      24.09
 H      -3.540443     6.192064     0.153850      20.88
 H      -2.337776     4.751979     0.911701      24.18
 C      -3.854345     3.471203    -3.185176      11.14
 O      -3.935256     4.743933    -3.798617     176.62
 H      -3.525283     5.234519    -3.095970      23.90
 C      -4.408503     2.298200    -3.765728      45.95
 H      -4.739174     1.997637    -4.734490      25.42
 C      -3.936263     1.041748    -1.561204      41.15
 C      -3.863424    -0.333453    -0.938465     107.52
 H      -4.402311    -1.039114    -1.494335      23.29
 O      -4.682597    -0.267867     0.256669     248.08
 H      -4.255642    -0.026071     1.050378      27.73
 C      -2.551151    -1.076885    -0.930830      73.27
 H      -1.975581    -1.024652    -1.961312      20.55
 C      -2.303383    -2.615447    -0.549828     102.31
 O      -3.520408    -3.362901    -0.880477     242.54
 H      -3.326393    -3.817780    -1.879074      27.06
 H      -1.919713    -2.644163     0.622233      22.93
 H      -1.469357    -2.937595    -1.029330      24.95
 C       1.869990    -0.728656    -0.965513      47.13
 H       2.580303    -1.137672    -1.703445      19.57
 C       1.710211     0.557373     1.109428      69.45
 H       2.277388     1.110671     1.834328      17.78
 C       0.317516     0.499838     1.089282      -1.43
 O      -0.603879     1.198990     1.885721     219.49
 C      -0.009397     1.665057     3.074743     108.63
 H       0.688874     2.696070     2.762262      21.30
 H      -0.818970     2.217068     3.734061      23.18
 H       0.569355     0.959327     3.593363      26.19
 C      -0.367540    -0.223511    -0.047876      16.19
 O      -1.656705    -0.207496     0.024439     121.84
 C       0.495345    -0.956344    -0.911620      71.24
 H       0.031173    -1.888102    -1.555546      18.36
 C       2.487614    -0.175940     0.066742      29.30
 C       4.135007    -0.052329     0.085546      53.14
 H       4.564906    -0.861493    -0.683983      18.67
 O       4.299715     1.370962    -0.039066     283.64
 H       5.185241     1.777678    -0.050790      24.65
 C       4.645423    -0.514032     1.563855     111.23
 H       4.325189     0.074022     2.386628      23.43
 O       4.162465    -1.925666     1.792589     284.75
 H       4.613956    -2.020107     2.679247      27.96
 C       6.155945    -0.441944     1.634228      87.03
 O       6.745389     0.828110     1.227927     327.45
 H       6.963358     1.318691     2.126916      28.10
 H       6.514101    -1.368473     1.091905      27.96
 H       6.763176    -0.653779     2.759876      25.93
55
name= lig-ACN-Water-frame_865
 C      -4.311792     1.144496    -2.940946      57.83
 H      -4.588885     0.085363    -3.287417      23.04
 C      -3.531912     2.331984    -1.028312      30.13
 H      -2.970558     2.328521     0.009354      14.00
 C      -3.552892     3.528459    -1.816985       3.78
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 O      -3.210247     4.712439    -1.301109     221.92
 C      -3.260831     4.891645     0.210441      55.17
 H      -4.087937     4.149516     0.553317      24.47
 H      -3.257015     6.075158     0.537859      22.22
 H      -2.222552     4.447100     0.375661      26.67
 C      -3.961775     3.461653    -3.197848      -7.25
 O      -3.964352     4.692340    -3.818769     205.73
 H      -3.250626     5.346925    -3.557625      27.90
 C      -4.394020     2.196660    -3.753470      64.53
 H      -4.734516     2.238650    -4.829212      20.75
 C      -3.878710     1.086447    -1.648131      28.39
 C      -3.920705    -0.274243    -0.949504      87.07
 H      -4.509626    -0.773589    -1.676809      26.32
 O      -4.707938    -0.280512     0.253839     210.71
 H      -3.990417    -0.186958     0.977877      25.13
 C      -2.364358    -1.006233    -0.935079      73.04
 H      -2.029759    -0.679744    -2.009207      22.20
 C      -2.305651    -2.622555    -0.544559      96.41
 O      -3.534854    -3.425761    -0.881727     277.56
 H      -3.415673    -3.603991    -1.787465      32.62
 H      -2.377759    -2.670577     0.623138      24.10
 H      -1.472419    -3.198865    -0.917696      24.03
 C       1.863679    -0.724066    -1.023260      43.62
 H       2.377743    -1.281495    -1.755013      21.38
 C       1.761251     0.554405     1.125503      72.29
 H       2.236423     1.324086     1.811659      17.74
 C       0.372955     0.598746     0.942639      13.72
 O      -0.487811     1.072855     1.893890     185.83
 C      -0.050144     1.774354     3.208108      73.29
 H       0.654510     2.785019     2.806969      20.20
 H      -0.999711     2.029377     3.868326      23.13
 H       0.655759     1.146382     3.719324      24.36
 C      -0.244344    -0.213113     0.015830      20.47
 O      -1.725101    -0.222128     0.064011     139.47
 C       0.477276    -0.967266    -0.870480      53.51
 H      -0.027953    -1.665357    -1.805484      18.90
 C       2.497274    -0.043294     0.151021      13.15
 C       4.075822    -0.010296     0.214401      79.79
 H       4.491095    -0.499227    -0.742877      20.61
 O       4.309732     1.484761    -0.104263     249.53
 H       5.252210     1.504278    -0.444678      24.94
 C       4.610776    -0.597973     1.552850     105.82
 H       4.115204     0.150095     2.164662      24.41
 O       4.152354    -1.868906     1.788440     333.70
 H       4.610140    -2.465472     2.303629      31.35
 C       6.100149    -0.604458     1.679191      72.03
 O       6.677688     0.799993     1.201263     324.85
 H       6.721481     1.573031     1.927359      26.79
 H       6.606434    -1.142696     0.853503      25.79
 H       6.388731    -0.861489     2.947431      23.74
55
name= lig-ACN-Water-frame_866
 C      -4.272835     1.035915    -3.061606      35.12
 H      -4.830651     0.159931    -3.579742      20.24
 C      -3.534052     2.413946    -0.965575      56.33
 H      -3.132977     2.469592     0.205884      14.24
 C      -3.534539     3.475419    -1.795187      22.00
 O      -3.235475     4.772268    -1.287648     212.15
 C      -3.140650     4.692874     0.163671     100.61
 H      -4.057024     4.307100     0.605625      27.58
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 H      -3.322117     5.866065     0.398768      23.94
 H      -2.319214     4.315729     0.794693      28.95
 C      -4.046226     3.487830    -3.113890      23.85
 O      -4.029104     4.652651    -3.955956     159.63
 H      -3.243147     5.119708    -3.494337      26.72
 C      -4.326990     2.332976    -3.787757      36.98
 H      -4.730458     2.382851    -4.883190      19.67
 C      -3.809144     1.184850    -1.655349       8.32
 C      -3.905664    -0.350295    -1.040525      72.38
 H      -4.449555    -1.170438    -1.575808      22.80
 O      -4.677098    -0.327802     0.308398     147.26
 H      -4.116099    -0.001858     1.155778      22.93
 C      -2.442398    -0.965940    -0.899536      75.39
 H      -1.894487    -0.798915    -1.904113      22.45
 C      -2.459535    -2.547238    -0.538433     107.22
 O      -3.497125    -3.441512    -0.927249     277.22
 H      -3.609959    -3.357232    -1.845455      31.58
 H      -2.401812    -2.579500     0.589495      25.63
 H      -1.429932    -2.909337    -0.847805      23.52
 C       1.916286    -0.759391    -0.884968      70.14
 H       2.445251    -0.973725    -1.739315      23.34
 C       1.802252     0.649073     1.103038      64.24
 H       2.233154     1.037941     2.123718      19.38
 C       0.399247     0.645411     1.007577       5.53
 O      -0.452504     1.057135     2.022793     192.96
 C      -0.059936     1.810578     3.179876      97.12
 H       0.319718     3.008204     3.039374      21.83
 H      -1.208863     1.847177     3.537389      21.53
 H       0.550626     1.241859     3.944504      23.07
 C      -0.291414    -0.248779     0.033197      -1.70
 O      -1.662323    -0.247630     0.119171     128.86
 C       0.480889    -0.896177    -0.976590      50.02
 H      -0.228537    -1.416087    -1.867141      19.67
 C       2.551882    -0.058519     0.041839      40.59
 C       4.000607     0.090134     0.188443      99.96
 H       4.476239    -0.607216    -0.540096      23.09
 O       4.386351     1.486465    -0.116397     246.97
 H       5.330381     1.337119    -0.328712      24.89
 C       4.542842    -0.443781     1.565710      87.82
 H       4.295204    -0.011424     2.554742      23.03
 O       4.031570    -1.966222     1.764232     252.61
 H       4.999012    -2.324855     1.816036      25.17
 C       6.221247    -0.513844     1.609193      79.11
 O       6.614463     0.696798     1.225752     370.47
 H       6.446815     1.280839     1.953480      31.29
 H       6.617451    -1.380999     1.035177      27.87
 H       6.484468    -1.057429     2.792373      24.55
55
name= lig-ACN-Water-frame_867
 C      -4.221572     1.156026    -3.076750      50.14
 H      -4.364430     0.133979    -3.565342      22.46
 C      -3.524752     2.207527    -1.068795      27.77
 H      -3.479083     2.195301     0.184174      17.79
 C      -3.579149     3.594889    -1.760934       2.35
 O      -3.219041     4.776451    -1.259865     219.11
 C      -3.113333     4.714311     0.212199      85.74
 H      -3.979164     4.274622     0.559488      27.01
 H      -2.874500     5.834719     0.627955      22.53
 H      -2.246522     4.111288     0.288954      26.02
 C      -4.021903     3.549596    -3.148887       6.57
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 O      -4.060581     4.621832    -4.015038     161.75
 H      -3.800422     5.477875    -3.742275      32.34
 C      -4.324545     2.312770    -3.788165      60.41
 H      -4.647794     2.334020    -4.901254      21.06
 C      -3.905221     0.980709    -1.730320      25.69
 C      -3.860577    -0.269972    -0.925290     108.01
 H      -4.465050    -0.814926    -1.750767      22.17
 O      -4.608933    -0.395190     0.283746     224.47
 H      -4.045647     0.102570     0.918555      26.07
 C      -2.594496    -1.017795    -0.873837      71.25
 H      -2.132532    -0.873023    -1.867091      23.09
 C      -2.510112    -2.433680    -0.457464     109.63
 O      -3.507163    -3.400650    -1.006431     205.15
 H      -3.388571    -3.465544    -2.115351      24.73
 H      -2.581252    -2.499189     0.576376      26.01
 H      -1.471271    -2.843405    -0.844976      22.03
 C       1.885428    -0.800338    -0.959084      34.48
 H       2.548138    -1.241124    -1.645004      22.74
 C       1.747225     0.690760     1.071930      64.03
 H       2.451129     1.060136     1.917619      18.65
 C       0.392218     0.507644     1.128471      20.42
 O      -0.456061     1.050378     2.076434     205.52
 C      -0.203653     1.841164     3.218154      95.44
 H       0.339417     3.036516     2.722722      21.56
 H      -1.008467     2.150495     3.948874      24.96
 H       0.729337     1.405125     3.812087      24.42
 C      -0.259220    -0.174448     0.036484      17.46
 O      -1.633304    -0.286870     0.177727     122.67
 C       0.496715    -0.746254    -0.999792      62.02
 H       0.236219    -1.459848    -1.900327      19.58
 C       2.486324     0.027722     0.134125      -2.01
 C       4.122890     0.079015     0.176939      88.30
 H       4.498944    -0.606150    -0.570229      24.07
 O       4.487947     1.444166    -0.125344     261.14
 H       5.429260     1.672160    -0.028142      24.25
 C       4.599754    -0.533891     1.626142      96.33
 H       4.175306     0.205492     2.417507      23.14
 O       3.994264    -1.917644     1.704396     266.52
 H       4.688188    -2.689376     1.536292      28.41
 C       6.051491    -0.620248     1.601051     100.73
 O       6.692813     0.758396     1.218093     314.23
 H       6.763075     1.307964     2.023596      29.32
 H       6.440409    -1.164818     0.731240      26.85
 H       6.752275    -0.607758     2.602661      24.01
55
name= lig-ACN-Water-frame_868
 C      -4.203823     1.047044    -3.144224      46.01
 H      -4.280193     0.216021    -3.862493      23.33
 C      -3.582729     2.259327    -1.188251      71.61
 H      -3.240394     2.114682    -0.037409      20.14
 C      -3.661011     3.447947    -1.798991       6.12
 O      -3.226042     4.810561    -1.217486     187.04
 C      -3.017616     4.757151     0.261322     100.54
 H      -3.888671     4.524433     0.677684      28.86
 H      -2.608637     5.744489     0.742489      24.29
 H      -2.389405     3.960948     0.549880      31.28
 C      -3.943841     3.563998    -3.182387      22.16
 O      -4.097156     4.673560    -4.080276     166.56
 H      -4.363524     5.374070    -3.422151      24.98
 C      -4.304645     2.335670    -3.750013      34.32
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 H      -4.501800     2.320056    -4.852994      25.24
 C      -3.936918     1.015872    -1.728213      25.95
 C      -3.976524    -0.321496    -0.971912      98.27
 H      -4.541482    -1.210579    -1.487500      22.38
 O      -4.580385    -0.398329     0.312017     237.55
 H      -4.033536    -0.215545     1.048684      26.74
 C      -2.486067    -0.946725    -0.861070      83.31
 H      -2.095469    -0.889005    -1.872487      25.57
 C      -2.560504    -2.520063    -0.383067     107.41
 O      -3.523430    -3.296078    -1.094301     205.52
 H      -3.039771    -3.721492    -2.046587      22.40
 H      -2.773297    -2.570294     0.573321      28.57
 H      -1.422117    -2.923127    -0.400903      24.23
 C       1.986435    -0.646797    -0.914026      60.27
 H       2.375685    -1.368447    -1.621506      23.84
 C       1.765101     0.690053     1.152333      52.32
 H       1.989681     1.609007     1.767553      22.59
 C       0.325016     0.435815     1.226479      -7.08
 O      -0.622649     0.974603     2.118501     113.89
 C      -0.130160     1.961323     3.224243      77.00
 H       0.234852     3.129846     2.586983      21.38
 H      -1.200558     1.972176     3.608139      24.00
 H       0.659498     1.443412     3.976219      24.20
 C      -0.256968    -0.141695     0.025548      -8.53
 O      -1.695445    -0.337908     0.163596     160.55
 C       0.484265    -0.678179    -1.024777      64.16
 H      -0.228188    -1.109014    -1.697351      23.90
 C       2.659310    -0.013558     0.054322      28.32
 C       4.090433    -0.013779     0.195877      97.56
 H       4.531532    -0.562740    -0.561355      26.06
 O       4.552492     1.440219    -0.123552     232.57
 H       5.259016     1.388118     0.566915      21.10
 C       4.551927    -0.604745     1.533500     100.47
 H       4.055542    -0.056436     2.477339      23.36
 O       3.954383    -1.829707     1.664030     330.56
 H       4.548632    -2.510158     1.565003      32.48
 C       6.135456    -0.610853     1.625966      64.59
 O       6.774202     0.861547     1.186565     204.87
 H       7.319928     1.224076     2.013694      25.19
 H       6.368545    -1.261150     0.784115      28.88
 H       6.253192    -1.472835     2.448201      25.89
55
name= lig-ACN-Water-frame_869
 C      -4.217170     0.970327    -3.214545      54.07
 H      -4.618207     0.063673    -3.640901      22.00
 C      -3.635197     2.297455    -1.079943      18.28
 H      -3.136427     2.483890    -0.081902      21.19
 C      -3.609377     3.636008    -1.854749      -8.29
 O      -3.269203     4.713654    -1.199762     157.93
 C      -2.970781     4.760577     0.330488     105.50
 H      -3.842590     4.968129     0.836405      26.62
 H      -2.509367     5.709375     0.196506      25.59
 H      -2.324762     4.085404     0.743066      30.22
 C      -3.972310     3.505983    -3.254541      26.41
 O      -4.134428     4.720605    -4.009388     134.44
 H      -4.425123     5.511854    -3.404888      28.75
 C      -4.225719     2.280160    -3.856056      67.36
 H      -4.549118     2.379063    -4.873987      23.57
 C      -3.994548     0.971137    -1.828740      -7.67
 C      -3.912978    -0.468099    -1.030830      72.94
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 H      -4.524955    -1.173766    -1.791457      21.29
 O      -4.637355    -0.369429     0.402623     150.74
 H      -3.905972    -0.071552     0.999523      25.22
 C      -2.431154    -1.015694    -0.885768      84.49
 H      -1.847148    -0.956120    -1.756232      25.29
 C      -2.593411    -2.532889    -0.340085     106.95
 O      -3.528594    -3.230046    -1.166461     214.97
 H      -3.181416    -3.547540    -2.089753      24.45
 H      -3.031974    -2.411261     0.482137      29.77
 H      -1.569365    -3.184924    -0.249272      24.18
 C       1.906689    -0.589528    -0.963876      28.26
 H       2.669586    -0.800687    -1.769525      21.13
 C       1.732340     0.635856     1.146048      70.26
 H       2.309330     1.273975     1.802803      21.19
 C       0.348921     0.463300     1.174495       9.73
 O      -0.642658     0.931486     2.190339     178.51
 C      -0.204906     1.956234     3.096766      98.23
 H       0.323191     3.216014     2.677928      22.19
 H      -0.965481     2.349020     3.826327      25.36
 H       0.631126     1.484729     3.818754      23.96
 C      -0.373473    -0.198502     0.115785      15.18
 O      -1.690544    -0.299771     0.140256     151.77
 C       0.497014    -0.598131    -1.001754      59.94
 H       0.295143    -1.020625    -1.881261      24.29
 C       2.517588     0.066629     0.177565      12.76
 C       4.128897     0.040984     0.110223      94.40
 H       4.391540    -0.693098    -0.549425      24.88
 O       4.596783     1.370159    -0.042209     259.97
 H       5.150807     1.791832     0.636787      24.72
 C       4.581017    -0.438588     1.481269      74.83
 H       4.336511     0.356375     2.346536      22.13
 O       3.897595    -1.897623     1.644426     238.77
 H       4.735135    -2.483615     1.651898      28.05
 C       6.218966    -0.576680     1.512176     107.18
 O       6.812136     0.743932     1.274342     294.72
 H       7.134365     1.310868     2.133892      28.51
 H       6.724029    -1.124474     0.726870      27.17
 H       6.774882    -0.557741     2.525521      22.91
55
name= lig-ACN-Water-frame_870
 C      -4.259621     1.027669    -3.173482      32.78
 H      -4.609953     0.155762    -3.735538      22.32
 C      -3.704322     2.234720    -1.210167      81.65
 H      -3.654275     2.052429    -0.183249      22.42
 C      -3.605137     3.389326    -1.830807      12.25
 O      -3.282944     4.721527    -1.145923     243.30
 C      -2.965262     4.889701     0.281174      95.15
 H      -3.830992     4.848156     0.937650      25.43
 H      -2.436576     5.759033     0.396076      26.70
 H      -2.421677     4.042008     0.514964      32.36
 C      -4.010843     3.528490    -3.241403     -10.81
 O      -4.173834     4.717821    -3.925398     177.03
 H      -3.993979     5.431177    -3.312839      26.53
 C      -4.184746     2.221726    -4.014893      38.76
 H      -4.579997     2.194689    -4.981974      22.04
 C      -3.917791     1.009603    -1.732176      34.22
 C      -3.850469    -0.362387    -0.989353      82.69
 H      -4.552617    -1.225730    -1.480600      21.39
 O      -4.623458    -0.362793     0.284728     206.19
 H      -4.230636     0.149376     1.130834      23.06
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 C      -2.447311    -1.146912    -0.889593      90.73
 H      -2.115304    -1.102092    -1.888399      24.68
 C      -2.645540    -2.502339    -0.362568     114.70
 O      -3.573073    -3.224389    -1.213689     290.48
 H      -3.333490    -3.249606    -2.067727      32.36
 H      -3.077280    -2.413463     0.493068      28.02
 H      -1.577966    -3.036418    -0.161204      24.05
 C       1.875918    -0.419095    -0.944690      48.37
 H       2.290076    -0.603199    -1.998722      20.27
 C       1.694715     0.631251     1.247963      67.65
 H       2.049595     0.728786     2.208025      17.04
 C       0.225741     0.535191     1.178909      -0.52
 O      -0.566197     0.899100     2.180395     192.32
 C      -0.196243     1.981716     3.058784      85.60
 H       0.232567     2.749454     2.019582      20.66
 H      -1.160631     2.196899     3.559413      23.96
 H       0.728385     1.680632     3.710318      23.19
 C      -0.262897    -0.256277     0.095512       7.75
 O      -1.766987    -0.226758     0.156857      99.20
 C       0.444002    -0.625492    -1.031010      57.52
 H      -0.105666    -0.924507    -1.846034      21.68
 C       2.490373     0.077287     0.161448      29.21
 C       4.019263     0.109747     0.172682     106.07
 H       4.323331    -0.296168    -0.690111      23.74
 O       4.606355     1.431659    -0.055377     246.55
 H       5.324513     1.394622     0.611567      21.37
 C       4.748345    -0.502023     1.453197      83.37
 H       4.270576     0.153938     2.320359      20.24
 O       3.981822    -1.821529     1.624374     264.60
 H       4.583146    -2.532267     2.179767      25.52
 C       6.270849    -0.513427     1.503334      79.39
 O       6.857972     0.744359     1.281105     415.19
 H       6.866627     1.189254     2.187663      31.91
 H       6.532579    -1.300496     0.824340      28.61
 H       6.386240    -1.211402     2.522107      25.38
55
name= lig-ACN-Water-frame_871
 C      -4.244431     1.064318    -3.167248      71.95
 H      -4.320830     0.087576    -3.703444      23.41
 C      -3.709535     2.101612    -1.058447      33.72
 H      -3.723459     2.330779    -0.106349      21.35
 C      -3.657242     3.404916    -1.869431     -33.08
 O      -3.340492     4.733779    -1.219386     168.10
 C      -2.990753     4.853974     0.210270     105.80
 H      -3.975198     4.971985     0.758166      23.36
 H      -2.668290     5.826186     0.340590      25.24
 H      -2.256417     4.201289     0.653863      29.46
 C      -3.988584     3.409731    -3.246247      35.20
 O      -4.180653     4.707703    -3.812858     193.78
 H      -3.551883     5.248660    -3.327099      27.80
 C      -4.214737     2.282411    -3.892545      89.01
 H      -4.353767     2.252552    -4.930330      23.14
 C      -3.889069     0.898091    -1.872648      13.03
 C      -3.904232    -0.299646    -0.983608     117.70
 H      -4.464760    -0.972961    -1.821979      23.62
 O      -4.627427    -0.315115     0.186450     216.82
 H      -3.978080     0.012583     0.948072      22.83
 C      -2.567459    -0.947771    -0.817689      94.38
 H      -1.989561    -1.011244    -1.718425      24.91
 C      -2.722904    -2.548761    -0.356491     108.63
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 O      -3.633167    -3.233241    -1.200898     261.19
 H      -3.315813    -3.502413    -2.048650      28.09
 H      -3.083467    -2.624310     0.613357      27.10
 H      -1.671934    -3.075017    -0.406211      24.31
 C       1.785996    -0.299336    -1.071818      12.57
 H       2.595546    -0.673547    -1.786934      20.78
 C       1.643645     0.517977     1.351544      58.79
 H       2.016814     0.897386     2.226844      20.75
 C       0.311117     0.468649     1.130786      25.00
 O      -0.604471     0.813327     2.196270     192.43
 C      -0.128590     2.038681     2.909759     113.41
 H       0.178728     3.248058     2.561181      22.39
 H      -1.075205     2.362716     3.445945      25.48
 H       0.516060     1.833731     3.778227      25.88
 C      -0.421924    -0.153802     0.104818      24.65
 O      -1.735138    -0.264487     0.076228     187.09
 C       0.394724    -0.626937    -1.026953      47.75
 H      -0.117074    -1.089245    -1.950080      20.78
 C       2.472536     0.183166     0.234597      -4.74
 C       4.039129     0.120703     0.185841      83.06
 H       4.198778    -0.628895    -0.482887      24.69
 O       4.569575     1.582574    -0.034755     227.93
 H       5.540974     1.555513     0.131407      21.47
 C       4.658764    -0.530846     1.442079      93.61
 H       4.585080     0.137976     2.402432      19.99
 O       4.177535    -1.772394     1.596133     307.12
 H       4.446063    -2.010531     2.474591      28.02
 C       6.224915    -0.711053     1.480886      86.64
 O       6.907448     0.768725     1.278239     299.80
 H       7.227321     1.214072     2.075932      30.92
 H       6.759415    -1.021850     0.601956      26.56
 H       6.697301    -1.115999     2.545367      25.33
55
name= lig-ACN-Water-frame_872
55
name= lig-ACN-Water-frame_873
 C      -4.093323     1.042702    -3.198782      71.97
 H      -4.348185    -0.002805    -3.587513      22.73
 C      -3.634484     2.086586    -1.007540      42.18
 H      -3.359463     2.247474    -0.071841      19.65
 C      -3.728905     3.432379    -1.745499      -9.86
 O      -3.414186     4.707527    -1.296133     218.10
 C      -3.182847     4.886375    -0.026562     109.13
 H      -4.200535     4.465341     0.580768      23.01
 H      -3.114872     5.913387     0.442276      23.74
 H      -2.228213     4.381613     0.331104      28.53
 C      -4.046699     3.359222    -3.099637      29.93
 O      -4.068135     4.684791    -3.731170     141.78
 H      -3.620767     5.245480    -3.033535      22.98
 C      -4.251519     2.296815    -3.829071      86.04
 H      -4.732052     2.396768    -4.842716      23.99
 C      -3.986424     0.972225    -1.866918      20.45
 C      -4.037780    -0.360672    -1.061009     101.56
 H      -4.731050    -0.805860    -1.744787      26.01
 O      -4.791642    -0.203676     0.163643     200.05
 H      -4.185879     0.229802     0.787125      26.81
 C      -2.620331    -1.100012    -0.980766      74.79
 H      -1.870004    -1.130965    -1.782609      23.66
 C      -2.709823    -2.492401    -0.453161     111.66
 O      -3.781688    -3.246033    -1.139067     147.18
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 H      -3.513084    -3.506658    -2.252715      21.62
 H      -3.053807    -2.305694     0.639046      25.97
 H      -1.773861    -3.040080    -0.475759      26.42
 C       1.898179    -0.284783    -1.044827      14.17
 H       2.514639    -0.406831    -1.908206      20.32
 C       1.599570     0.458776     1.255049      56.45
 H       1.976685     0.588050     2.331808      20.44
 C       0.276548     0.327671     1.251629      15.61
 O      -0.676887     0.849891     2.262988     185.08
 C      -0.141886     2.090365     2.840070     114.49
 H       0.049609     3.059871     2.176190      25.24
 H      -1.074644     2.613771     3.250755      25.61
 H       0.552770     2.145921     3.574847      28.30
 C      -0.449722    -0.085278     0.090027     -33.89
 O      -1.907718    -0.235579     0.151850      59.49
 C       0.438411    -0.466113    -1.117850      27.03
 H      -0.065600    -1.004353    -2.150591      21.77
 C       2.582699     0.193002     0.171027      12.93
 C       4.052975     0.291440     0.148632      88.65
 H       4.270152    -0.466390    -0.572166      24.39
 O       4.397786     1.688892     0.014327     251.74
 H       5.387152     1.769321    -0.018510      24.01
 C       4.772136    -0.415816     1.488817      93.25
 H       4.668916     0.011353     2.481446      23.35
 O       4.274787    -1.851210     1.626396     230.56
 H       5.046756    -2.365190     2.204217      23.60
 C       6.209748    -0.532293     1.327515      88.19
 O       7.037682     0.657354     1.128894     273.20
 H       7.002467     1.361754     1.932465      28.56
 H       6.476175    -0.814170     0.205692      25.12
 H       6.615359    -1.241074     2.215824      26.45
55
name= lig-ACN-Water-frame_874
 C      -4.177020     1.056883    -3.167799      39.35
 H      -4.319463     0.222738    -3.920969      22.19
 C      -3.633204     2.179275    -1.079712      82.97
 H      -3.575744     1.925759    -0.039899      26.08
 C      -3.708637     3.312153    -1.769352      13.31
 O      -3.457074     4.750614    -1.399639     170.92
 C      -3.239386     4.942770     0.199082      63.49
 H      -4.163383     4.327927     0.804796      23.22
 H      -3.267853     6.137007     0.124706      23.09
 H      -2.251156     4.392514     0.507370      27.14
 C      -4.123977     3.507394    -3.159799      11.60
 O      -4.020450     4.665533    -3.740304     127.90
 H      -3.900152     5.341593    -3.084663      27.62
 C      -4.270643     2.239847    -3.913284      23.25
 H      -4.545184     2.196619    -5.035726      17.67
 C      -3.881656     0.947272    -1.709652      22.48
 C      -4.104484    -0.336068    -1.055825     102.47
 H      -4.580024    -1.090838    -1.527442      26.90
 O      -4.814286    -0.219910     0.158562     171.10
 H      -4.500097     0.503084     0.855847      26.78
 C      -2.628536    -1.028264    -0.983605      74.40
 H      -2.433267    -0.775846    -2.075446      26.30
 C      -2.734406    -2.562944    -0.483238     109.05
 O      -3.779557    -3.213720    -1.106363     201.15
 H      -3.559852    -3.419234    -2.153968      24.09
 H      -3.098878    -2.581610     0.656237      25.90
 H      -1.807909    -3.077574    -0.471302      27.91
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 C       1.878415    -0.295262    -1.087686      60.69
 H       2.453112    -0.545481    -1.906969      24.90
 C       1.697898     0.485178     1.274472      46.46
 H       2.219678     0.720980     2.326639      18.64
 C       0.126235     0.398966     1.199265     -35.57
 O      -0.611060     0.837160     2.289698     201.45
 C      -0.220560     2.189803     2.799039     106.79
 H       0.285918     2.643414     1.926128      24.96
 H      -1.106507     2.487038     3.471304      24.69
 H       0.531834     1.850810     3.383542      25.55
 C      -0.505457    -0.222378     0.067544      13.31
 O      -1.864055    -0.276830     0.054045     135.70
 C       0.472398    -0.359466    -1.024663      34.14
 H      -0.117792    -0.328895    -2.119898      24.99
 C       2.424931     0.078940     0.172380      28.06
 C       4.035750     0.205638     0.281819      84.56
 H       4.534087    -0.099620    -0.648717      22.88
 O       4.349389     1.771260     0.042709     210.08
 H       5.327035     1.853136     0.077594      24.01
 C       4.648274    -0.452924     1.477832     116.24
 H       4.342606     0.193204     2.255337      25.52
 O       4.281158    -1.761318     1.594994     285.83
 H       5.103551    -2.372892     1.874173      26.20
 C       6.276742    -0.550750     1.175239      72.35
 O       7.178463     0.791499     1.049750     196.74
 H       7.247297     1.087174     2.080085      27.39
 H       6.399707    -1.327810     0.217590      26.57
 H       6.867797    -1.108089     1.999629      27.56
55
name= lig-ACN-Water-frame_875
 C      -4.260875     1.008071    -3.168629      74.70
 H      -4.415800    -0.026347    -3.488924      23.20
 C      -3.656012     2.221974    -1.065503      35.07
 H      -3.387350     2.554289     0.028432      18.34
 C      -3.715135     3.531808    -1.844343       3.74
 O      -3.475697     4.664965    -1.296880     161.26
 C      -3.329722     5.001727     0.226431      61.42
 H      -4.384445     4.663486     0.823508      22.09
 H      -3.280884     6.219624     0.282330      21.20
 H      -2.231631     4.530608     0.611542      24.42
 C      -4.086458     3.403682    -3.208306      18.60
 O      -4.027361     4.756864    -3.857227     135.66
 H      -3.916157     5.423652    -3.124957      25.00
 C      -4.313034     2.238218    -3.882888      79.46
 H      -4.239381     2.250689    -5.007024      24.17
 C      -3.907070     1.042485    -1.860242      -6.75
 C      -4.041461    -0.435378    -1.020035      86.64
 H      -4.605812    -0.944873    -1.633159      27.99
 O      -4.878567    -0.259064     0.242779     167.80
 H      -4.353536     0.396301     0.742665      28.08
 C      -2.700951    -1.014809    -0.881429      97.31
 H      -2.112505    -1.118036    -1.868902      23.27
 C      -2.706729    -2.498735    -0.477151     101.08
 O      -3.831798    -3.238628    -1.165845     257.57
 H      -3.472772    -3.636516    -1.904540      30.78
 H      -2.776557    -2.541342     0.760288      24.42
 H      -1.838205    -2.901971    -0.777104      27.72
 C       1.764932    -0.290136    -0.964948      45.29
 H       2.171682    -0.435573    -1.917823      22.85
 C       1.532282     0.440191     1.264771      54.52
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 H       2.094726     1.188690     2.000808      21.06
 C       0.235727     0.422124     1.200501      15.40
 O      -0.620877     0.829375     2.274517     240.28
 C      -0.215506     2.147086     2.827388     128.68
 H      -0.104344     2.861706     1.992308      27.63
 H      -1.047961     2.840321     3.176950      25.30
 H       0.617699     2.307956     3.419481      28.23
 C      -0.381691    -0.244856     0.050289       8.72
 O      -1.805110    -0.305536    -0.066535     154.07
 C       0.360596    -0.279072    -1.115730      50.57
 H      -0.089009    -0.446290    -2.187164      22.84
 C       2.475597     0.010559     0.173769      32.96
 C       3.925607     0.257707     0.195940      78.76
 H       4.349315    -0.361833    -0.722016      22.77
 O       4.260373     1.725415     0.144085     228.54
 H       5.235167     1.774798     0.242445      26.04
 C       4.765615    -0.270161     1.456565      80.86
 H       4.628073     0.115589     2.397452      25.61
 O       4.207217    -1.790930     1.535308     276.80
 H       4.740027    -2.230339     2.183441      29.53
 C       6.475336    -0.420216     1.105031      77.20
 O       7.180527     0.767349     1.016437     315.99
 H       7.343422     1.085692     1.920680      31.21
 H       6.369746    -0.991226     0.022014      25.98
 H       6.677433    -0.996888     1.972395      28.14
55
name= lig-ACN-Water-frame_876
 C      -4.315803     0.975496    -3.172380      30.50
 H      -4.665332     0.158621    -3.769368      22.26
 C      -3.685941     2.314874    -1.186307      62.91
 H      -3.293599     2.097325    -0.069201      17.22
 C      -3.776240     3.480357    -1.799121       9.56
 O      -3.472959     4.775342    -1.138812     234.71
 C      -3.428732     5.046040     0.147028      83.75
 H      -4.438033     4.732944     0.791877      22.84
 H      -3.142471     6.231728     0.232322      21.04
 H      -2.687918     4.343038     0.877779      24.83
 C      -3.997774     3.554858    -3.262525       5.37
 O      -4.083200     4.721093    -3.985073     145.13
 H      -3.723951     5.432261    -3.279188      23.79
 C      -4.309402     2.233130    -3.909849      11.21
 H      -4.669921     2.264578    -4.962476      22.60
 C      -4.009071     1.026551    -1.700824      16.81
 C      -4.074403    -0.248608    -1.026367      97.40
 H      -4.565428    -0.982214    -1.561401      25.81
 O      -4.842075    -0.276941     0.237825     210.22
 H      -4.363060    -0.090522     1.021096      28.09
 C      -2.624583    -1.124430    -0.919436      59.84
 H      -2.390919    -1.045477    -2.056202      23.35
 C      -2.709283    -2.574408    -0.477402     106.58
 O      -3.826548    -3.242992    -1.176622     271.68
 H      -3.438752    -3.658355    -1.889596      30.44
 H      -2.902689    -2.779330     0.755574      22.73
 H      -1.823921    -2.970781    -0.712231      26.94
 C       1.724695    -0.303107    -1.055505      38.17
 H       2.562286    -0.406540    -1.752916      19.84
 C       1.647856     0.505628     1.268874      63.24
 H       1.940399     1.031294     2.237234      17.71
 C       0.158066     0.292305     1.205211      -1.43
 O      -0.638747     0.866932     2.277728     227.50
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 C      -0.257595     2.225749     2.754989     101.94
 H       0.024051     2.800161     1.940449      27.55
 H      -1.126418     2.190326     3.436434      24.14
 H       0.526104     1.993431     3.453505      24.72
 C      -0.453131    -0.128254    -0.013497      16.12
 O      -1.769150    -0.221828     0.022960     144.55
 C       0.327079    -0.318095    -1.208288      61.73
 H      -0.160881    -0.783630    -2.060474      23.72
 C       2.394406     0.052574     0.247823      27.06
 C       3.952891     0.277035     0.190864      69.82
 H       4.291111    -0.230343    -0.847869      21.37
 O       4.141909     1.676166     0.213209     248.72
 H       5.114541     1.830527     0.342679      24.78
 C       4.902900    -0.348179     1.338291      91.55
 H       4.747346     0.311539     2.125822      26.39
 O       4.213142    -1.685934     1.495580     325.92
 H       4.351738    -1.982672     2.395216      30.17
 C       6.377831    -0.417700     1.101302     113.15
 O       7.202883     0.832801     1.024880     332.03
 H       7.221218     1.295156     1.844703      34.59
 H       6.770508    -0.810535     0.058345      24.81
 H       6.952964    -1.094228     1.619306      27.13
55
name= lig-ACN-Water-frame_877
 C      -4.368331     1.144464    -3.131322      77.13
 H      -4.692528     0.232359    -3.554185      24.51
 C      -3.695664     2.195843    -1.110395      27.52
 H      -3.486155     2.312293     0.061289      17.16
 C      -3.782502     3.637745    -1.839383     -10.17
 O      -3.492595     4.823259    -1.323576     164.33
 C      -3.545506     5.060941     0.343317      49.91
 H      -4.661518     5.075759     0.547523      22.69
 H      -3.141426     6.166184     0.383532      20.62
 H      -2.700104     4.250941     0.816901      20.48
 C      -3.991357     3.530512    -3.231129      13.97
 O      -4.134817     4.683597    -4.059668     196.53
 H      -3.664143     5.491655    -3.813150      28.10
 C      -4.299057     2.314315    -3.833564      75.14
 H      -4.806471     2.305626    -4.789500      24.80
 C      -4.126040     1.040690    -1.804229      20.59
 C      -4.061956    -0.340819    -0.955512     104.10
 H      -4.707209    -0.864617    -1.646873      22.80
 O      -4.780488    -0.238801     0.251127     240.68
 H      -3.995994    -0.287946     0.934404      22.91
 C      -2.642967    -0.944890    -0.934011      64.19
 H      -2.054845    -0.894866    -1.936363      21.36
 C      -2.715582    -2.722710    -0.467166      87.26
 O      -3.783577    -3.275646    -1.169582     231.11
 H      -3.580839    -3.380497    -2.222726      24.94
 H      -3.144826    -2.550270     0.716158      21.72
 H      -1.866240    -3.266590    -0.498528      25.40
 C       1.842898    -0.281993    -1.059361      46.47
 H       2.203654    -0.749448    -2.050594      20.27
 C       1.537906     0.532621     1.379943      69.21
 H       2.206540     0.577001     2.197619      17.89
 C       0.210757     0.343127     1.245321       9.67
 O      -0.656813     0.820373     2.183844     214.06
 C      -0.328463     2.152779     2.778786     108.30
 H      -0.270120     2.936282     2.113159      26.64
 H      -1.077043     2.757869     3.298280      24.81
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 H       0.695041     2.191396     3.240226      24.35
 C      -0.446633    -0.017464    -0.084692     -12.78
 O      -1.921723    -0.205988     0.072927     150.44
 C       0.382679    -0.460048    -1.166569      55.50
 H      -0.003418    -0.728843    -2.052353      22.59
 C       2.393482     0.099225     0.113421      17.18
 C       3.980655     0.211527     0.160277      74.56
 H       4.442744     0.062598    -0.913221      19.31
 O       4.064531     1.739801     0.244866     258.05
 H       5.011216     2.000898     0.295085      24.07
 C       4.809909    -0.384288     1.240126     101.21
 H       4.717374     0.198516     2.107952      22.21
 O       4.276174    -1.588355     1.494889     262.09
 H       4.563324    -2.011731     2.462914      24.37
 C       6.446804    -0.533285     0.970974      71.32
 O       7.152280     0.962867     1.077986     279.74
 H       7.178689     1.113357     2.078931      29.59
 H       6.379384    -1.046300    -0.037483      27.54
 H       6.657109    -1.049452     1.777458      29.94
55
name= lig-ACN-Water-frame_878
 C      -4.471125     1.127775    -3.117115      32.57
 H      -4.774887     0.307747    -3.772813      21.75
 C      -3.773774     2.389222    -1.078379      80.73
 H      -3.718570     2.337111     0.043937      23.05
 C      -3.713763     3.511192    -1.776031      11.71
 O      -3.509313     4.915729    -1.361926     193.24
 C      -3.631997     5.087179     0.259672      67.86
 H      -4.603099     4.842932     0.573641      26.29
 H      -3.135150     6.022766     0.636029      23.81
 H      -3.139066     4.046589     0.875920      24.51
 C      -4.045901     3.573890    -3.198527      21.76
 O      -4.179181     4.644700    -4.142449     167.77
 H      -3.648625     5.312702    -3.717238      26.59
 C      -4.369062     2.448713    -3.849771      35.22
 H      -4.418969     2.528599    -4.943493      25.29
 C      -4.073654     1.093582    -1.703384      -8.48
 C      -4.118081    -0.387343    -1.112147      77.02
 H      -4.631523    -1.350126    -1.500138      21.79
 O      -4.674349    -0.221357     0.332307     168.99
 H      -4.057510     0.255547     1.075342      22.56
 C      -2.636402    -0.954285    -0.874705      76.39
 H      -2.163341    -0.837371    -1.924653      24.84
 C      -2.748881    -2.559714    -0.463424      87.76
 O      -3.795746    -3.373213    -1.188269     164.68
 H      -3.411943    -3.345410    -2.294787      22.66
 H      -3.146006    -2.646048     0.761491      22.70
 H      -1.816544    -2.993981    -0.516526      26.91
 C       1.770245    -0.360136    -1.074888      24.94
 H       2.641516    -0.548257    -1.882754      21.76
 C       1.688421     0.349348     1.202927      42.61
 H       1.855880     0.732960     2.144069      19.84
 C       0.169035     0.503862     1.094469     -32.71
 O      -0.736259     0.822906     2.207891     172.99
 C      -0.377056     2.151892     2.728141     114.76
 H      -0.346342     2.669314     1.904974      28.77
 H      -1.150934     2.081449     3.487004      23.97
 H       0.604951     2.150657     3.373158      22.91
 C      -0.482923    -0.043034     0.002046       6.63
 O      -1.894409    -0.168623     0.095816     130.80
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 C       0.390651    -0.499472    -1.069910      74.10
 H       0.008199    -0.827016    -1.899538      27.70
 C       2.481018     0.143373     0.144160      24.86
 C       3.917604     0.402755     0.022387      93.05
 H       4.243394    -0.284645    -0.886149      22.92
 O       4.032175     1.820184     0.262247     205.68
 H       4.997129     2.008515     0.294377      24.74
 C       4.834398    -0.250355     1.245232      57.88
 H       4.805885     0.421985     2.087005      23.14
 O       4.277520    -1.731347     1.545120     223.43
 H       5.079425    -2.049818     2.109830      26.40
 C       6.412977    -0.410471     0.927223     115.35
 O       6.978841     0.853005     1.068901     297.06
 H       7.251774     1.186343     2.045088      28.61
 H       7.034997    -0.686679     0.082762      25.19
 H       6.853348    -1.050928     1.549688      28.99
55
name= lig-ACN-Water-frame_879
 C      -4.491218     1.198478    -3.106574      69.51
 H      -4.729718     0.186282    -3.535594      24.78
 C      -3.878286     2.349351    -1.022778      27.43
 H      -3.683519     2.432115     0.006124      23.75
 C      -3.716911     3.721688    -1.836714      -9.30
 O      -3.520880     4.918397    -1.230031     219.45
 C      -3.708272     4.998076     0.044459     107.34
 H      -4.708777     4.998003     0.260906      26.43
 H      -3.419982     5.992753     0.275278      23.80
 H      -2.771772     4.269458     0.651959      24.65
 C      -4.118841     3.620073    -3.217951       9.32
 O      -4.139847     4.671378    -4.088607     148.37
 H      -3.965518     5.649235    -3.796227      27.35
 C      -4.461942     2.300186    -3.850027      63.81
 H      -4.571251     2.286388    -4.969724      21.95
 C      -4.112767     1.099444    -1.765991      15.38
 C      -4.049798    -0.216815    -0.940965      96.37
 H      -4.852114    -0.701042    -1.699574      23.33
 O      -4.613402    -0.246828     0.343763     230.26
 H      -4.107527     0.409231     0.818356      28.63
 C      -2.708448    -1.028823    -0.938271      73.37
 H      -2.160178    -1.090719    -1.927836      24.68
 C      -2.804157    -2.396381    -0.463235     101.90
 O      -3.746648    -3.364780    -1.164524     172.66
 H      -3.223697    -3.952803    -1.959145      23.44
 H      -3.111663    -2.484386     0.794719      23.50
 H      -1.835482    -2.808974    -0.583278      26.36
 C       1.769013    -0.394039    -0.990310      56.70
 H       2.144308    -0.628050    -2.136352      23.25
 C       1.554541     0.394294     1.208671      53.44
 H       2.230678     0.707993     1.924592      22.42
 C       0.181393     0.527996     1.069415      18.35
 O      -0.630092     0.792453     2.147631     240.65
 C      -0.487103     2.121402     2.744659     118.55
 H      -0.561477     2.984133     2.329890      31.02
 H      -1.211342     2.448405     3.487956      27.11
 H       0.640030     2.070038     3.124201      24.33
 C      -0.478732    -0.162964    -0.002986      11.37
 O      -1.825652    -0.154263     0.084406      83.18
 C       0.308264    -0.534523    -1.063057      70.70
 H      -0.114372    -1.103903    -1.783132      27.53
 C       2.427117     0.042619     0.053055      28.93
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 C       3.988109     0.441000     0.103004      76.85
 H       4.417526     0.588069    -0.977149      21.21
 O       4.065668     1.929412     0.190635     214.75
 H       5.019537     2.168874     0.316186      25.97
 C       4.845403    -0.361858     1.159825      94.41
 H       4.586442     0.191398     2.075456      23.37
 O       4.342547    -1.706844     1.567775     306.73
 H       4.953164    -2.299335     1.848221      33.06
 C       6.322876    -0.397085     0.919027     109.96
 O       6.902177     0.942125     1.059538     342.81
 H       6.882222     1.162258     2.099773      27.82
 H       6.136805    -0.685668    -0.076085      27.49
 H       6.707261    -1.038543     1.558025      30.20
55
name= lig-ACN-Water-frame_880
 C      -4.453094     1.068240    -3.031996      36.42
 H      -4.744818     0.107667    -3.587954      21.93
 C      -3.886788     2.497863    -1.155561      97.86
 H      -3.649970     2.418181    -0.201478      22.76
 C      -3.912731     3.592524    -1.871797      25.11
 O      -3.487831     4.888277    -1.417495     199.66
 C      -3.768037     5.052851     0.160387      85.78
 H      -4.605608     4.514442     0.431459      29.14
 H      -3.652855     6.044864     0.364884      24.06
 H      -2.971971     4.347228     0.915059      23.96
 C      -4.157040     3.572198    -3.249425      23.93
 O      -4.106150     4.767977    -4.075566     117.81
 H      -4.099363     5.419974    -3.304273      25.41
 C      -4.500871     2.371138    -3.839918      24.59
 H      -5.075465     2.300224    -4.819241      21.83
 C      -4.125557     1.264175    -1.650353      21.94
 C      -4.046400    -0.079286    -0.951107      86.90
 H      -4.753016    -0.957649    -1.467681      21.27
 O      -4.623568    -0.232981     0.381854     263.85
 H      -4.120264    -0.032390     1.161798      26.43
 C      -2.750811    -0.870885    -1.029752      75.33
 H      -2.332738    -0.748485    -2.061261      25.12
 C      -2.812853    -2.491075    -0.419834      86.30
 O      -3.675992    -3.305550    -1.081651     278.60
 H      -3.179119    -3.650999    -1.772858      29.10
 H      -3.232710    -2.222031     0.778315      23.09
 H      -1.781213    -2.847823    -0.259335      24.23
 C       1.657332    -0.495688    -1.154170      30.51
 H       2.360980    -0.884855    -2.088956      22.10
 C       1.664077     0.551716     1.181573      62.06
 H       1.791731     0.872752     2.207305      18.35
 C       0.217070     0.382051     1.132296      12.46
 O      -0.605194     0.848770     2.111748     229.24
 C      -0.513944     2.145039     2.816818      88.80
 H      -0.737231     2.648121     2.052722      29.48
 H      -1.226215     1.811868     3.579592      24.28
 H       0.510179     2.416916     3.313603      24.39
 C      -0.451921    -0.180960    -0.017611      13.58
 O      -1.881815    -0.249936    -0.008923     141.50
 C       0.301585    -0.685301    -1.126571      61.51
 H      -0.132730    -1.124527    -2.033454      23.91
 C       2.394294     0.046270     0.104454      12.58
 C       3.970455     0.378839     0.062043      54.95
 H       4.428318    -0.261051    -0.856076      22.20
 O       4.099148     2.033639     0.194846     147.37
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 H       5.061475     2.112692     0.432437      21.71
 C       4.706191    -0.366740     1.302584      90.79
 H       4.736525     0.316550     2.201199      23.18
 O       4.313063    -1.688250     1.470970     242.30
 H       5.177063    -2.002958     1.952475      26.11
 C       6.216408    -0.437127     0.829201      93.87
 O       6.840970     1.083725     1.014299     263.98
 H       7.116796     1.225755     1.971039      29.18
 H       6.607462    -0.711496    -0.090204      29.39
 H       6.784789    -1.011395     1.380517      31.14
55
name= lig-ACN-Water-frame_881
 C      -4.435211     1.176316    -3.047575      70.42
 H      -4.729970     0.161900    -3.421432      23.98
 C      -3.846474     2.516239    -1.039562      26.37
 H      -3.553889     2.821947    -0.120751      17.01
 C      -3.989157     3.708607    -1.971410      -8.25
 O      -3.519230     4.863008    -1.465520     165.67
 C      -3.786288     5.059453     0.204138      70.14
 H      -4.710638     4.584216     0.285955      29.10
 H      -3.985571     6.038076     0.366531      23.87
 H      -2.633680     4.782044     0.688759      20.91
 C      -4.207222     3.602614    -3.381923      15.59
 O      -4.111169     4.800525    -3.975890     195.79
 H      -3.857587     5.473995    -3.383172      24.18
 C      -4.601022     2.256943    -3.839153      63.08
 H      -4.996335     2.355434    -4.871548      22.16
 C      -4.169322     1.190556    -1.668107      15.89
 C      -4.137226    -0.161648    -0.917335      75.46
 H      -4.828770    -0.786846    -1.732937      20.88
 O      -4.706844    -0.178318     0.454253     271.84
 H      -3.878977     0.085611     0.940088      24.68
 C      -2.657173    -0.849339    -1.010606      85.24
 H      -2.324094    -0.758990    -2.054720      23.10
 C      -2.772412    -2.309165    -0.385354      85.23
 O      -3.643831    -3.340258    -1.040428     271.74
 H      -3.561700    -3.307621    -1.929961      32.09
 H      -3.363957    -2.229720     0.718566      21.71
 H      -1.736413    -2.744235    -0.225737      23.57
 C       1.765422    -0.545791    -1.093707      38.82
 H       2.517380    -0.955550    -1.893057      22.33
 C       1.632065     0.577823     1.135500      50.88
 H       2.356882     1.154613     1.775052      17.56
 C       0.230797     0.301410     1.085804       8.18
 O      -0.628917     0.808563     2.135523     221.38
 C      -0.573762     2.084386     2.803261     112.08
 H      -0.929184     2.997560     2.486694      26.01
 H      -1.210355     2.161580     3.725585      25.25
 H       0.517952     2.184767     3.100042      25.35
 C      -0.477182    -0.250695    -0.095028      -1.22
 O      -1.835844    -0.269322    -0.042685     176.93
 C       0.308629    -0.790231    -1.162046      49.18
 H      -0.382944    -1.172009    -2.060945      21.16
 C       2.382533     0.133349     0.004509      24.45
 C       3.802439     0.302064     0.123872      81.82
 H       4.339621     0.007115    -0.914746      20.64
 O       4.144784     1.893013     0.161919     172.26
 H       5.069199     1.948878     0.484403      22.77
 C       4.709751    -0.173652     1.263557      73.60
 H       4.521614     0.298858     2.306209      22.96
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 O       4.253700    -1.745687     1.389718     214.45
 H       4.536791    -2.203360     2.337274      26.65
 C       6.305346    -0.213631     0.869291     106.40
 O       6.728615     1.088209     0.919333     345.91
 H       7.240700     1.222308     1.677008      32.74
 H       6.286256    -0.523620    -0.104581      30.80
 H       6.666849    -0.836054     1.512458      30.27
55
name= lig-ACN-Water-frame_882
 C      -4.499980     1.194884    -3.007773      33.41
 H      -4.716892     0.257320    -3.518788      24.11
 C      -3.887945     2.469187    -1.110152      69.48
 H      -3.649924     2.335962    -0.065962      18.85
 C      -3.903376     3.610802    -1.874267      12.63
 O      -3.599311     4.966397    -1.350674     257.58
 C      -3.767061     5.089523    -0.021952      94.22
 H      -4.361686     4.425156     0.603044      27.51
 H      -3.842544     6.156976     0.132568      23.44
 H      -2.729977     4.719023     0.716787      24.12
 C      -4.275881     3.596148    -3.266886      10.56
 O      -4.153605     4.848911    -4.025424     183.16
 H      -3.526435     5.370833    -3.444868      23.95
 C      -4.646765     2.375721    -3.966927      36.02
 H      -4.666623     1.958187    -4.914724      23.43
 C      -4.144001     1.222337    -1.599916      25.55
 C      -4.172099    -0.222067    -0.883052      80.58
 H      -4.975186    -1.047873    -1.316972      21.10
 O      -4.751310    -0.122816     0.391354     263.62
 H      -4.414759     0.398618     1.193438      23.42
 C      -2.753513    -0.932790    -0.964945      76.38
 H      -2.240967    -0.967618    -1.918937      23.66
 C      -2.792672    -2.265091    -0.404689      97.60
 O      -3.601818    -3.326001    -0.987291     213.96
 H      -3.552686    -3.219849    -2.088174      25.11
 H      -3.080100    -2.012871     0.757000      22.39
 H      -1.677534    -2.630193    -0.386332      23.81
 C       1.783166    -0.657379    -1.065256      48.10
 H       2.337294    -0.964429    -1.932364      23.21
 C       1.504072     0.562082     1.020475      67.75
 H       1.839635     1.258241     1.869872      19.65
 C       0.154396     0.419398     1.082465       6.08
 O      -0.722712     0.699267     2.101308     210.84
 C      -0.532328     2.050482     2.823208     105.59
 H      -0.825909     2.780199     2.114229      25.40
 H      -1.006630     1.735912     3.791494      23.31
 H       0.516242     2.137738     3.059304      23.91
 C      -0.373313    -0.324336    -0.084989      -4.21
 O      -1.748042    -0.159193    -0.005207      88.62
 C       0.424146    -0.777379    -1.113323      61.59
 H       0.204625    -1.532502    -2.067332      19.16
 C       2.315429     0.160534    -0.033718      39.95
 C       3.890385     0.404496     0.077263      82.31
 H       4.261188    -0.108107    -0.982301      22.24
 O       4.127428     1.694692     0.113613     249.42
 H       5.086204     1.867557     0.340654      20.21
 C       4.673901    -0.327039     1.235175      90.97
 H       4.283306     0.286012     2.167353      23.19
 O       4.240746    -1.690187     1.329796     331.18
 H       4.036840    -1.683825     2.246465      30.12
 C       6.136944    -0.162494     0.954193     116.61
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 O       6.752501     1.255324     0.813426     298.45
 H       6.885074     1.558394     1.776127      29.45
 H       6.369411    -0.578802     0.039134      29.10
 H       6.814383    -0.579616     1.534077      28.91
55
name= lig-ACN-Water-frame_883
 C      -4.613051     1.201254    -3.085181      76.99
 H      -4.769128     0.265943    -3.540021      24.18
 C      -3.874293     2.386991    -1.032805      41.41
 H      -3.637211     2.644895     0.079727      19.89
 C      -3.852880     3.631053    -1.829724      -6.80
 O      -3.719378     4.914614    -1.444771     183.16
 C      -3.644663     5.154560     0.074124      90.83
 H      -4.620192     4.670021     0.305424      25.24
 H      -3.850461     6.262641     0.314470      23.73
 H      -2.501256     4.829268     0.285094      24.48
 C      -4.280496     3.656700    -3.224565      10.91
 O      -4.197703     4.800915    -4.042905     154.42
 H      -3.534117     5.507316    -3.677901      25.90
 C      -4.531669     2.413851    -3.788752      48.51
 H      -4.613111     2.724460    -4.803150      20.19
 C      -4.211838     1.115847    -1.750298       9.36
 C      -4.129704    -0.119456    -0.893374      95.88
 H      -4.718771    -0.834371    -1.671497      24.44
 O      -4.854511    -0.080469     0.393632     242.11
 H      -4.064471     0.326020     0.908914      25.37
 C      -2.775951    -0.849023    -0.897732      81.83
 H      -2.660556    -0.778732    -1.974649      26.00
 C      -2.733336    -2.420540    -0.293458      88.45
 O      -3.607958    -3.267933    -0.955818     177.25
 H      -3.118038    -3.555972    -1.990795      22.83
 H      -3.112796    -2.552657     0.799593      23.90
 H      -1.589610    -2.777252    -0.322505      23.06
 C       1.924120    -0.662722    -1.069907      45.45
 H       2.550810    -1.095763    -1.785401      23.61
 C       1.484901     0.688006     1.043176      61.49
 H       1.978013     1.073763     1.986760      22.02
 C       0.075445     0.423813     0.997106       9.35
 O      -0.749685     0.654724     2.094026     202.59
 C      -0.450586     1.883219     2.797033     132.30
 H      -0.933039     2.677313     2.275710      28.09
 H      -1.125244     2.025034     3.672692      25.21
 H       0.511774     2.166525     2.990040      28.85
 C      -0.438312    -0.314696    -0.062980       2.21
 O      -1.830846    -0.119485    -0.084390     130.10
 C       0.419655    -0.880159    -1.094138      30.90
 H      -0.354631    -1.446822    -1.891720      22.90
 C       2.418607     0.104938     0.010502      11.41
 C       3.875000     0.242127    -0.074828      95.11
 H       4.445861    -0.329677    -0.971390      20.74
 O       4.134943     1.770669     0.055101     189.88
 H       5.152799     1.837652     0.093571      18.13
 C       4.519987    -0.305015     1.188285      94.50
 H       4.385369     0.219779     2.231104      21.87
 O       4.234758    -1.699828     1.317681     302.63
 H       3.732721    -1.999394     2.078726      30.85
 C       6.160433    -0.223110     0.993087      67.32
 O       6.717163     1.455416     0.750663     154.38
 H       6.788136     1.827909     1.749319      25.16
 H       6.519791    -0.601760     0.098010      27.77
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 H       6.448769    -0.534311     1.923350      28.21
55
name= lig-ACN-Water-frame_884
 C      -4.641907     1.160065    -3.178747      28.79
 H      -5.081632     0.418776    -3.813754      19.03
 C      -3.850555     2.411956    -1.120589      78.43
 H      -3.608697     2.199900     0.049798      19.16
 C      -3.932905     3.619389    -1.814832      27.81
 O      -3.779537     4.979844    -1.441636     189.27
 C      -3.567673     5.215082     0.115035      73.20
 H      -4.230872     4.677939     0.888295      24.76
 H      -3.447895     6.396495     0.125333      22.99
 H      -2.604902     4.666878     0.708722      23.92
 C      -4.130489     3.626796    -3.145076      40.26
 O      -4.242980     4.720374    -4.035275     172.56
 H      -3.853168     5.448027    -3.563300      27.13
 C      -4.470180     2.487046    -3.776578      31.77
 H      -4.988804     2.314720    -4.712366      21.43
 C      -4.225076     1.230705    -1.715727     -18.39
 C      -4.211880    -0.167042    -0.964464      81.52
 H      -4.885172    -0.993853    -1.437506      22.75
 O      -4.878827    -0.008917     0.354070     265.39
 H      -4.399072     0.171441     1.185590      26.05
 C      -2.790833    -0.924393    -0.828799      90.15
 H      -2.289469    -1.143307    -1.749894      23.94
 C      -2.695653    -2.421783    -0.200929      88.40
 O      -3.635314    -3.307774    -1.014816     209.87
 H      -3.067665    -3.715980    -1.796772      25.69
 H      -2.925851    -2.351204     0.895286      24.81
 H      -1.573809    -2.879595    -0.334676      22.88
 C       1.806235    -0.674715    -1.029539      41.93
 H       2.499087    -1.071513    -1.770249      24.35
 C       1.597680     0.662102     1.017519      79.73
 H       2.118986     1.248244     1.781559      22.61
 C       0.237581     0.406289     1.031286     -11.29
 O      -0.694277     0.630562     2.061196     210.83
 C      -0.480073     1.869780     2.805842     121.33
 H      -0.576215     2.688506     2.245583      29.10
 H      -0.866729     1.613989     3.788712      25.82
 H       0.498384     1.645417     3.045127      27.04
 C      -0.538691    -0.276472    -0.203730      -7.62
 O      -1.893462    -0.069610    -0.168499     164.69
 C       0.318983    -0.950704    -1.043674      49.70
 H       0.018514    -1.436522    -2.122267      23.44
 C       2.353460     0.051663     0.022256      35.42
 C       3.858195     0.280888    -0.036442      84.28
 H       4.149059    -0.010593    -1.109468      22.74
 O       4.143282     1.809506    -0.097578     185.57
 H       5.113733     1.927703     0.126868      20.08
 C       4.630692    -0.209448     1.154826      84.59
 H       4.016267     0.420749     1.923461      22.47
 O       4.247948    -1.827109     1.278643     177.77
 H       3.607272    -1.892761     2.154107      27.56
 C       6.182793    -0.063283     1.080049      94.70
 O       6.587114     1.446014     0.756361     233.65
 H       7.072691     1.622091     1.631084      24.00
 H       6.500330    -0.821909     0.397601      27.90
 H       6.775887    -0.370713     1.942200      27.12
55
name= lig-ACN-Water-frame_885
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 C      -4.539731     1.258916    -3.097818      73.45
 H      -4.975050     0.276406    -3.394620      24.59
 C      -3.842551     2.410036    -1.151500      32.04
 H      -3.490293     2.442106     0.023882      18.14
 C      -3.946482     3.728259    -1.756927     -17.43
 O      -3.798414     5.043462    -1.179196     216.48
 C      -3.444492     5.243854     0.095267     107.53
 H      -4.434420     5.128246     0.674104      22.82
 H      -3.199022     6.433445     0.252937      20.30
 H      -2.356326     4.702818     0.109580      24.49
 C      -4.076914     3.538581    -3.292684     -11.66
 O      -4.239169     4.704666    -3.987536     166.78
 H      -4.204720     5.485881    -3.405060      24.14
 C      -4.570107     2.305115    -3.942191      63.44
 H      -4.803839     2.605737    -4.975138      24.09
 C      -4.232467     1.112461    -1.799562      28.22
 C      -4.282266    -0.257004    -0.929543      79.14
 H      -4.995864    -0.860095    -1.549993      24.07
 O      -4.916368     0.042271     0.301071     294.60
 H      -4.170452     0.286512     0.851511      26.20
 C      -2.828402    -1.104790    -0.926247      58.23
 H      -2.662165    -1.144398    -1.991419      22.77
 C      -2.804070    -2.399244    -0.216357     105.45
 O      -3.600715    -3.342849    -0.981518     282.18
 H      -3.276651    -3.388563    -1.807648      33.87
 H      -3.197350    -2.480569     0.736857      25.37
 H      -1.570251    -2.718011    -0.163876      23.05
 C       1.615810    -0.731447    -0.966620      48.00
 H       2.098589    -1.036006    -1.978087      24.42
 C       1.627354     0.569056     1.036009      58.30
 H       1.923683     1.343986     1.689400      22.32
 C       0.178666     0.292290     0.946942      27.68
 O      -0.644488     0.628371     1.974818     184.87
 C      -0.344970     1.794807     2.925947     124.92
 H      -0.601300     2.622926     2.462473      29.07
 H      -1.218214     1.853147     3.522810      26.72
 H       0.552983     2.052047     3.376779      27.37
 C      -0.451949    -0.143756    -0.120516       9.01
 O      -1.857738     0.037454    -0.147669      79.47
 C       0.247223    -0.937395    -1.141589      30.62
 H      -0.165420    -1.529205    -2.005673      22.19
 C       2.373668     0.061342    -0.025440       9.72
 C       3.867517     0.464365    -0.123101     107.87
 H       4.366390    -0.232181    -0.886862      24.48
 O       4.087070     1.811365    -0.284688     225.15
 H       4.858147     1.992986     0.295860      20.23
 C       4.685991    -0.287551     1.186691      82.85
 H       4.437268     0.062540     2.286368      21.66
 O       4.341870    -1.756342     1.229454     297.95
 H       3.940420    -1.653455     2.086729      28.19
 C       6.193918     0.059852     1.163836     103.37
 O       6.484701     1.318359     0.809593     320.08
 H       7.039591     1.719862     1.431579      30.32
 H       6.640049    -0.440846     0.310570      25.15
 H       6.578132    -0.216343     2.225246      25.30
55
name= lig-ACN-Water-frame_886
 C      -4.549152     1.055472    -3.164441      25.74
 H      -4.726641     0.075365    -3.772551      19.33
 C      -3.849188     2.428052    -1.091514      56.81
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 H      -3.626547     2.519093     0.066741      17.27
 C      -3.896747     3.636971    -1.859529      10.48
 O      -3.898987     4.963020    -1.254063     186.77
 C      -3.260654     5.300847     0.203607      58.65
 H      -3.864446     4.946264     1.124706      23.60
 H      -2.942333     6.449404     0.126360      22.59
 H      -2.429962     4.561874     0.697480      21.99
 C      -4.198908     3.578571    -3.247717      21.09
 O      -4.209241     4.753037    -4.010496     140.17
 H      -4.155215     5.496132    -3.266146      24.15
 C      -4.508083     2.384299    -3.964689      38.50
 H      -4.718340     2.204718    -5.012147      25.01
 C      -4.079881     1.160193    -1.676432       5.03
 C      -4.284270    -0.232874    -1.007192      94.94
 H      -4.936955    -0.921227    -1.511332      25.86
 O      -4.903569     0.029267     0.274987     282.94
 H      -4.389916     0.513932     1.003855      24.66
 C      -2.946917    -0.926979    -0.959201      71.27
 H      -2.493150    -1.033151    -1.939627      22.23
 C      -2.898295    -2.416220    -0.221169     100.83
 O      -3.570424    -3.415288    -0.960810     266.96
 H      -3.446706    -3.333314    -1.881209      30.72
 H      -3.383720    -2.210350     0.628586      26.02
 H      -1.776763    -2.840601     0.144525      23.26
 C       1.708066    -0.734412    -1.074875      31.10
 H       2.422845    -1.128603    -1.979360      23.87
 C       1.544566     0.488161     1.023824      71.74
 H       2.042678     0.878044     1.869743      23.15
 C       0.213443     0.350875     1.030528       5.87
 O      -0.611534     0.712677     2.065609     234.95
 C      -0.339342     1.783793     2.953028     126.36
 H      -0.253366     2.536611     2.379522      29.66
 H      -1.068157     1.672858     3.682604      25.95
 H       0.558319     1.432128     3.513110      25.21
 C      -0.596132    -0.212068    -0.185561       1.92
 O      -1.899673     0.009815    -0.198268     129.75
 C       0.151997    -0.809256    -1.143109      60.94
 H      -0.487894    -1.279400    -1.801412      23.38
 C       2.351690     0.060722    -0.127366      13.29
 C       3.910619     0.288390    -0.117124      77.56
 H       4.365141    -0.073417    -1.044615      24.29
 O       4.014976     1.889585    -0.443542     157.83
 H       4.766819     2.213295     0.101131      22.85
 C       4.643411    -0.237135     1.218004      95.50
 H       4.144764     0.316002     2.127562      21.40
 O       4.477384    -1.605415     1.169164     315.47
 H       4.270899    -2.182774     1.882757      29.97
 C       6.213923    -0.161325     1.182824      73.56
 O       6.430781     1.449663     0.845234     281.56
 H       6.812813     1.707513     1.753284      25.52
 H       6.778088    -0.938110     0.616228      26.53
 H       6.610529    -0.419471     2.293254      25.39
55
name= lig-ACN-Water-frame_887
 C      -4.380865     1.148045    -3.136602      85.84
 H      -4.609392     0.167431    -3.710435      22.85
 C      -3.855712     2.385184    -1.092719      64.30
 H      -3.770606     2.414276    -0.000303      21.03
 C      -3.895437     3.576304    -1.841585      -8.50
 O      -3.926610     4.826070    -1.309946     125.34
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 C      -3.143035     5.205986     0.238994      68.89
 H      -4.030886     5.383143     0.869049      23.39
 H      -2.816986     6.242458    -0.126672      24.19
 H      -2.096189     4.627118     0.059930      20.62
 C      -4.318179     3.608654    -3.249278      -0.59
 O      -4.195621     4.808225    -4.012671     200.16
 H      -3.859273     5.608150    -3.577761      26.98
 C      -4.412847     2.285751    -3.772734      52.42
 H      -4.644301     2.439023    -4.796506      20.72
 C      -4.115195     1.173120    -1.862231      39.28
 C      -4.218536    -0.053420    -0.990006      99.96
 H      -4.850097    -0.618013    -1.553271      27.54
 O      -4.924461    -0.054285     0.286002     254.50
 H      -4.350515     0.512321     0.929755      25.51
 C      -2.845466    -0.891928    -0.915297      94.36
 H      -2.590472    -1.004334    -1.986407      25.39
 C      -3.021620    -2.258643    -0.206856      84.81
 O      -3.600460    -3.502606    -0.964275     163.78
 H      -3.054494    -3.585640    -1.939805      24.23
 H      -3.531309    -2.265201     0.597360      27.03
 H      -1.798927    -2.507201     0.038095      23.15
 C       1.641092    -0.634703    -1.253357      44.85
 H       2.270571    -1.028955    -2.245225      22.27
 C       1.618437     0.425962     0.964035      58.76
 H       2.081821     0.616250     1.918688      19.30
 C       0.034348     0.393309     1.001529       3.16
 O      -0.721200     0.718086     2.124656     205.21
 C      -0.226380     1.764138     3.063258     131.93
 H       0.032815     2.648435     2.766006      30.99
 H      -1.034052     2.042142     3.633628      25.97
 H       0.686177     1.512564     3.661241      25.62
 C      -0.592605    -0.188483    -0.057372      -4.40
 O      -2.082792    -0.041397    -0.206958     132.98
 C       0.321813    -0.752093    -1.217424      52.00
 H       0.086108    -1.170268    -2.062825      25.03
 C       2.355946    -0.021809    -0.126991      19.17
 C       3.858464     0.253745    -0.174458      87.83
 H       4.314932    -0.346597    -0.922665      25.11
 O       3.932330     1.851592    -0.483546     166.26
 H       4.873328     2.062001    -0.196671      19.15
 C       4.672376    -0.094168     1.138700      99.56
 H       4.220104     0.491682     2.012622      21.79
 O       4.524257    -1.669601     1.072930     199.89
 H       4.614891    -1.771485     2.156234      25.60
 C       6.150293    -0.090495     1.217434      83.47
 O       6.439623     1.429514     0.945301     323.91
 H       6.824043     1.791188     1.899504      24.82
 H       6.483993    -0.616344     0.250719      25.08
 H       6.723795    -0.246970     2.285489      24.94
55
name= lig-ACN-Water-frame_888
 C      -4.217556     1.149101    -3.183016      24.05
 H      -4.546328     0.134840    -3.632308      22.64
 C      -3.861630     2.398318    -1.164731      74.97
 H      -3.688693     2.345158    -0.153956      22.83
 C      -4.017373     3.592554    -1.810903      35.29
 O      -3.843967     4.843519    -1.176799     277.23
 C      -3.127395     5.126382    -0.107575     113.58
 H      -3.626434     4.899663     0.844568      24.41
 H      -2.742926     6.142205    -0.144474      25.04
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 H      -2.392601     4.210171     0.411686      21.98
 C      -4.217430     3.643038    -3.168202      27.19
 O      -4.222552     4.739608    -4.019794     224.54
 H      -3.747343     5.319276    -3.438358      25.35
 C      -4.402830     2.476207    -3.930373      37.68
 H      -4.534895     2.356014    -4.953568      25.47
 C      -4.126505     1.149275    -1.692132      16.08
 C      -4.238822    -0.156734    -1.017348     105.30
 H      -4.823044    -0.757406    -1.554735      27.08
 O      -4.915759    -0.088112     0.280311     278.28
 H      -4.441749     0.443262     0.964460      26.34
 C      -2.956956    -0.925150    -0.998841      73.09
 H      -2.426583    -1.110863    -1.960333      23.13
 C      -3.094258    -2.284054    -0.250320      95.39
 O      -3.571748    -3.436699    -0.940193     186.73
 H      -2.865418    -3.707746    -1.838763      22.55
 H      -3.631635    -2.073800     0.574290      26.07
 H      -1.950543    -2.582342     0.199824      22.99
 C       1.712640    -0.422882    -1.283595      32.54
 H       2.141837    -0.646706    -2.401085      22.64
 C       1.429744     0.338485     0.982984      67.97
 H       2.018221     0.931600     1.723567      22.01
 C       0.114699     0.380043     0.993267      -1.15
 O      -0.802809     0.764539     2.152186     116.57
 C      -0.112858     1.784505     3.204263      99.91
 H       0.144451     2.342518     2.446289      27.42
 H      -0.990785     2.051506     3.705137      26.02
 H       0.577643     1.227912     3.945113      24.25
 C      -0.551662    -0.230989    -0.200683     -11.88
 O      -1.985348    -0.033813    -0.079002      85.02
 C       0.204310    -0.636594    -1.230062      78.33
 H      -0.433337    -0.961843    -1.913081      26.28
 C       2.352688    -0.093685    -0.139533      12.54
 C       3.827845     0.339510    -0.224840     101.89
 H       4.255385    -0.120652    -1.068005      23.78
 O       3.884538     1.665311    -0.451521     287.07
 H       4.837265     1.949928    -0.443274      24.07
 C       4.594928    -0.149341     1.034327     105.87
 H       4.117199     0.038151     1.989915      22.97
 O       4.497211    -1.674242     1.097063     238.64
 H       4.810930    -1.973333     2.007401      28.94
 C       6.117108     0.210652     1.076036      81.68
 O       6.503229     1.442686     1.031621     299.04
 H       6.976818     1.748447     2.011573      21.72
 H       6.728898    -0.414298     0.254989      25.02
 H       6.329086    -0.623352     1.915245      24.26
55
name= lig-ACN-Water-frame_889
 C      -4.226999     1.243135    -3.215228      77.67
 H      -4.244622     0.359622    -3.890174      24.74
 C      -3.884359     2.411228    -0.995005      32.63
 H      -3.616673     2.606233    -0.014239      20.45
 C      -4.067408     3.677085    -1.779228     -22.22
 O      -3.909824     4.912084    -1.304620     205.40
 C      -2.965428     4.982668    -0.019594     100.05
 H      -3.678721     5.111321     0.759475      22.83
 H      -2.431820     5.893240    -0.158306      24.23
 H      -2.049202     4.255095    -0.479237      21.03
 C      -4.147080     3.576588    -3.292664      -5.64
 O      -4.221231     4.752716    -3.960895     209.84
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 H      -3.980218     5.724402    -3.719095      20.39
 C      -4.311378     2.369842    -3.943579      83.13
 H      -4.386876     2.555262    -4.966156      28.37
 C      -4.116173     1.151370    -1.849729      21.73
 C      -4.357107    -0.316474    -1.038833      88.03
 H      -4.967942    -0.907966    -1.544457      27.28
 O      -4.909083    -0.125562     0.262847     281.88
 H      -4.273404     0.384298     0.783916      26.87
 C      -2.902875    -0.985818    -0.962638      56.88
 H      -2.573867    -0.892825    -2.040964      22.52
 C      -3.023495    -2.316459    -0.185417      96.08
 O      -3.561689    -3.375619    -0.957619     213.66
 H      -3.140402    -3.386108    -1.976935      24.80
 H      -3.811831    -2.219714     0.535592      24.24
 H      -1.937245    -2.581300     0.410583      23.49
 C       1.518505    -0.344689    -1.362091      43.20
 H       2.318021    -0.335741    -2.198931      24.20
 C       1.514254     0.348003     1.048263      47.94
 H       1.896669     0.885656     1.982023      22.03
 C       0.007986     0.288594     1.075283      10.06
 O      -0.733026     0.807690     2.110748     184.76
 C      -0.112413     1.698659     3.168943     109.32
 H       0.605247     2.502586     2.980651      26.22
 H      -0.787208     2.256626     3.820247      25.49
 H       0.575253     0.959044     3.691936      24.40
 C      -0.602252    -0.112429    -0.123613      11.81
 O      -1.898525    -0.139476    -0.040069     134.27
 C       0.140818    -0.500298    -1.354739      59.52
 H      -0.229335    -0.861507    -2.298036      23.04
 C       2.229192    -0.026586    -0.132809       7.76
 C       3.756589     0.119089    -0.244028      97.28
 H       4.124296    -0.388161    -1.070478      28.82
 O       3.857954     1.687816    -0.412050     223.44
 H       4.789024     1.997166    -0.362918      21.58
 C       4.508795    -0.280849     1.012921     107.43
 H       4.097306     0.390962     1.711163      24.43
 O       4.459405    -1.658566     1.083865     289.95
 H       4.837885    -1.900390     1.877551      31.59
 C       6.049469     0.061965     0.913657      78.72
 O       6.590770     1.709823     1.032487     164.14
 H       6.961603     1.777782     2.023781      20.50
 H       6.466368    -0.332810    -0.155238      23.04
 H       6.663021    -0.023221     1.866235      21.45
55
name= lig-ACN-Water-frame_890
 C      -4.274938     1.123410    -3.241987      25.53
 H      -4.325235     0.127234    -3.655955      22.34
 C      -4.010261     2.379439    -1.089527      82.37
 H      -3.989182     2.167630    -0.026714      22.10
 C      -4.009964     3.586759    -1.843374      13.53
 O      -3.975923     5.005874    -1.435070      95.13
 C      -2.777898     4.957913    -0.011081      30.50
 H      -3.152938     4.617440     0.889649      24.31
 H      -2.427828     5.920417    -0.083693      24.42
 H      -2.135073     3.815085    -0.087137      20.74
 C      -4.132373     3.643322    -3.200593       6.55
 O      -4.227919     4.807493    -4.031722     142.59
 H      -4.166059     5.398658    -3.184678      23.84
 C      -4.156860     2.425304    -3.991769      29.17
 H      -4.208361     2.253401    -5.058260      20.12
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 C      -4.128956     1.176699    -1.762865       8.36
 C      -4.296320    -0.213957    -1.091967      84.86
 H      -4.840261    -0.843757    -1.662760      26.94
 O      -4.923218    -0.173530     0.228798     244.93
 H      -4.311448     0.198607     0.937745      25.26
 C      -2.799838    -1.035678    -0.860060      94.50
 H      -2.307068    -1.350435    -1.848952      23.53
 C      -2.940705    -2.331373    -0.111403      87.45
 O      -3.564553    -3.368192    -1.040489     200.67
 H      -3.241250    -3.265595    -1.917507      29.94
 H      -3.479830    -2.113119     0.870137      25.06
 H      -1.787452    -2.756667     0.295442      23.87
 C       1.451051    -0.265051    -1.323548      51.51
 H       1.780699    -0.618531    -2.296230      24.32
 C       1.483350     0.377438     1.118424      73.81
 H       2.262242     0.367727     1.921910      20.00
 C       0.161884     0.289187     1.105541       0.23
 O      -0.698673     0.899127     2.071816     160.75
 C      -0.009816     1.553313     3.153623     102.30
 H       0.638099     2.337059     2.623778      25.27
 H      -1.038685     1.853108     3.544965      23.53
 H       0.307442     0.804552     3.958188      26.41
 C      -0.587601    -0.107826    -0.171373     -33.92
 O      -2.099761    -0.233837    -0.047516     148.41
 C       0.056743    -0.304913    -1.377223      59.71
 H      -0.591172    -0.578451    -2.328950      21.57
 C       2.110417     0.048966    -0.158331      15.97
 C       3.601433     0.048606    -0.276894      92.86
 H       3.973407    -0.487285    -1.078750      26.18
 O       3.849513     1.686289    -0.403838     124.58
 H       4.696453     1.790933     0.094854      22.20
 C       4.552567    -0.175118     0.984312     104.63
 H       4.224732     0.036906     1.920712      26.75
 O       4.407656    -1.747147     1.104235     161.62
 H       4.725436    -1.930090     2.103430      27.39
 C       6.086972     0.148491     0.831842      67.46
 O       6.517271     1.806500     0.835490     121.39
 H       7.044958     1.925560     1.735819      21.68
 H       6.462637    -0.132344    -0.310055      24.91
 H       6.625430    -0.698401     1.432538      26.88
55
name= lig-ACN-Water-frame_891
 C      -4.222767     1.130713    -3.193131      81.88
 H      -4.547163     0.329033    -3.785771      27.12
 C      -4.148947     2.384271    -1.198370      43.74
 H      -4.273209     2.626493    -0.079583      22.05
 C      -3.984278     3.660730    -1.897965     -43.54
 O      -3.858853     4.937360    -1.268235     190.08
 C      -2.784831     4.902071    -0.150600     100.48
 H      -3.431614     4.790801     0.627052      24.27
 H      -2.263828     5.818918     0.006919      25.72
 H      -1.762797     4.269958    -0.695993      22.95
 C      -4.119912     3.568384    -3.390430      -3.21
 O      -4.214443     4.798729    -3.961748     217.28
 H      -4.152510     5.633927    -3.577709      26.42
 C      -4.071914     2.296342    -3.928342      77.85
 H      -4.043722     2.480494    -5.024448      21.15
 C      -4.196240     1.100505    -1.842490      52.91
 C      -4.096831    -0.213398    -1.061611     104.48
 H      -4.765339    -0.742581    -1.685807      27.52
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 O      -4.946999    -0.229062     0.166272     231.67
 H      -4.453481     0.263773     0.938380      26.24
 C      -2.863940    -1.074953    -0.871140      75.01
 H      -2.255744    -1.173180    -1.813562      24.07
 C      -2.912221    -2.495510    -0.154450     100.64
 O      -3.591278    -3.317670    -1.002642     226.00
 H      -3.114133    -3.438149    -1.710042      33.96
 H      -3.486457    -2.573479     0.903437      24.68
 H      -1.700671    -2.844341    -0.101960      24.57
 C       1.375904    -0.217622    -1.381517      61.39
 H       2.089556    -0.430324    -2.091606      25.06
 C       1.537774     0.317958     1.044401      74.32
 H       1.913645     0.612852     2.034068      21.46
 C       0.044382     0.370468     0.995755       6.11
 O      -0.675643     0.866626     1.969304     180.76
 C      -0.051879     1.446303     3.206753      99.01
 H       0.957893     2.116411     2.951442      23.61
 H      -0.540609     2.276863     3.873483      23.84
 H       0.565802     0.690654     3.750079      26.40
 C      -0.764120    -0.085316    -0.061898      36.59
 O      -2.034067    -0.132066     0.068813     142.23
 C      -0.093565    -0.131925    -1.315261      40.99
 H      -0.792346    -0.227215    -2.334072      23.49
 C       2.122409     0.027571    -0.153407      26.47
 C       3.629568     0.278094    -0.193746     109.53
 H       3.942369    -0.141251    -1.104504      28.78
 O       3.858282     1.595563    -0.440135     235.47
 H       4.347144     2.072990     0.275655      26.34
 C       4.539453    -0.253187     0.965064      86.21
 H       4.239331     0.381490     1.725866      27.87
 O       4.435331    -1.756337     1.141206     238.69
 H       4.352372    -2.027313     2.175541      26.27
 C       6.121276     0.326016     0.625135      79.06
 O       6.388875     1.667992     0.684459     214.41
 H       6.822988     1.925102     1.608400      24.84
 H       6.343062     0.010095    -0.553259      24.37
 H       6.843323    -0.111904     1.459615      25.38
55
name= lig-ACN-Water-frame_892
 C      -4.171144     1.074343    -3.286023      25.09
 H      -4.153679     0.118394    -3.779677      21.86
 C      -4.214372     2.490549    -1.237477      61.44
 H      -4.053647     2.452869    -0.063788      21.05
 C      -4.033951     3.640570    -1.925610      37.85
 O      -3.763086     4.776389    -1.205613     278.49
 C      -2.792710     4.910845    -0.279584      94.48
 H      -2.772255     4.457175     0.681560      26.70
 H      -2.692260     6.001115    -0.299154      24.69
 H      -1.772079     4.037140    -0.475360      23.98
 C      -4.016833     3.624135    -3.271076      18.24
 O      -4.215393     4.739734    -4.072763     201.99
 H      -3.785285     5.395571    -3.456154      26.14
 C      -4.062735     2.330335    -4.014143      32.96
 H      -4.103030     2.014114    -5.097840      20.02
 C      -4.163665     1.144533    -1.798323     -18.83
 C      -4.230537    -0.370417    -1.039529      90.73
 H      -4.533123    -1.175342    -1.678440      25.96
 O      -4.946031    -0.266460     0.124267     286.90
 H      -4.521729     0.420238     0.702515      27.12
 C      -2.815151    -0.974118    -0.765201      84.23
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 H      -2.406276    -0.993064    -1.792768      23.50
 C      -2.834201    -2.488718    -0.226999      86.91
 O      -3.704028    -3.396303    -1.021598     215.64
 H      -3.327420    -3.551984    -1.916729      28.03
 H      -3.272432    -2.498571     0.917136      23.90
 H      -1.647681    -2.886111    -0.009681      24.48
 C       1.314660    -0.132259    -1.348522      44.61
 H       1.470934    -0.052296    -2.325541      24.63
 C       1.341112     0.315197     0.983651      59.93
 H       1.947134     0.804037     1.682097      22.95
 C       0.033267     0.440909     0.992056      20.91
 O      -0.751134     0.913902     2.092856     196.10
 C       0.053468     1.363649     3.205583      97.14
 H       0.990854     2.047392     2.936249      23.60
 H      -0.898992     1.864902     3.730486      23.33
 H       0.124608     0.419591     3.827984      25.31
 C      -0.681038     0.006172    -0.111522      18.35
 O      -2.134625    -0.060143     0.209410      98.91
 C      -0.051300    -0.071644    -1.312653      51.41
 H      -0.586254    -0.021305    -2.410536      23.12
 C       2.166186    -0.030568    -0.200896     -16.23
 C       3.727173     0.216456    -0.246288      89.19
 H       4.154631    -0.310985    -1.068752      26.47
 O       3.880529     1.745577    -0.488935     187.06
 H       4.065421     2.134454     0.383410      28.17
 C       4.598806    -0.240177     0.939613     111.54
 H       4.442900     0.057774     1.923301      26.27
 O       4.490492    -1.645997     1.167924     301.55
 H       4.219385    -1.657462     2.034990      31.50
 C       6.087142     0.193550     0.476721      77.55
 O       6.228556     1.713113     0.589385     204.20
 H       6.491807     1.815934     1.506040      28.08
 H       6.344816    -0.206340    -0.653942      24.48
 H       6.936299    -0.430963     1.039151      26.51
55
name= lig-ACN-Water-frame_893
 C      -4.065442     1.111689    -3.238204      74.53
 H      -3.919059     0.155113    -3.748314      24.63
 C      -4.164401     2.246711    -1.131446      46.33
 H      -4.139532     2.393206     0.035796      19.40
 C      -4.033194     3.507412    -1.874910     -27.70
 O      -3.871481     4.748070    -1.309013     183.04
 C      -2.571664     4.858908    -0.191593      81.09
 H      -3.024489     4.550500     0.728611      22.71
 H      -2.434770     6.001012    -0.053889      23.74
 H      -1.598366     4.724838    -1.036055      20.86
 C      -4.017656     3.514722    -3.415286     -23.34
 O      -4.137923     4.699767    -4.171010     194.34
 H      -3.854782     5.683274    -3.893288      20.20
 C      -4.093469     2.321492    -4.017168      71.39
 H      -4.082788     2.650628    -5.094032      26.65
 C      -4.175200     1.055362    -1.882655      37.53
 C      -4.294019    -0.356441    -1.113720      92.56
 H      -5.062916    -0.922380    -1.689584      23.77
 O      -5.040785    -0.304666     0.181479     266.35
 H      -4.590306     0.328439     0.738851      27.57
 C      -2.806806    -0.903905    -0.733158      89.43
 H      -2.110667    -0.865841    -1.524234      24.07
 C      -2.808622    -2.396344    -0.275379      79.05
 O      -3.745396    -3.411793    -1.012971     141.18
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 H      -3.320416    -3.302834    -2.035115      25.05
 H      -3.249331    -2.406357     0.910405      22.24
 H      -1.747910    -2.931673    -0.493841      23.20
 C       1.399723    -0.022439    -1.458255      48.94
 H       2.054770    -0.076184    -2.235596      28.85
 C       1.490304     0.396801     0.950826      42.78
 H       2.005929     0.458757     1.846229      24.21
 C      -0.064160     0.484150     1.092499      -4.97
 O      -0.749197     0.955201     2.138729     172.68
 C      -0.025358     1.251896     3.328167     110.14
 H       0.973705     1.900597     2.986751      25.02
 H      -0.530731     2.089985     4.017182      24.05
 H       0.501496     0.466602     3.897780      26.74
 C      -0.829137     0.152111    -0.078035       5.69
 O      -2.142133    -0.073536     0.192779     160.16
 C      -0.061592    -0.058272    -1.348487      40.51
 H      -0.711494    -0.208727    -2.309027      22.31
 C       2.156478    -0.019822    -0.241523      21.03
 C       3.648569     0.167725    -0.317162      56.61
 H       4.037034    -0.207219    -1.283399      27.47
 O       3.855624     1.843535    -0.546263      88.70
 H       4.198443     2.131616     0.325184      22.41
 C       4.717094    -0.133030     0.913927      94.94
 H       4.510689     0.667047     1.621964      24.69
 O       4.547524    -1.587371     1.163103     265.16
 H       4.291641    -1.835028     2.089194      28.12
 C       6.073266     0.012547     0.388601      74.85
 O       6.112258     1.719550     0.542923      47.10
 H       6.466984     1.924949     1.419711      25.54
 H       6.081050     0.100640    -0.739410      23.06
 H       6.810124    -0.666731     1.001107      25.51
55
name= lig-ACN-Water-frame_894
 C      -3.976135     1.074664    -3.331031      35.08
 H      -4.144626     0.178817    -4.004647      23.47
 C      -4.071150     2.144564    -1.141039      51.07
 H      -4.303338     2.106879    -0.048901      21.39
 C      -3.982551     3.390043    -1.914415      -9.39
 O      -3.871360     4.783759    -1.276890     192.48
 C      -2.552116     4.919534    -0.295712      55.28
 H      -2.620009     4.019400     0.382666      22.83
 H      -2.600599     5.997857     0.196495      22.21
 H      -1.520166     4.313051    -0.735859      22.06
 C      -4.095561     3.543482    -3.286553     -12.03
 O      -4.038944     4.606410    -4.258375     187.94
 H      -4.152781     5.401473    -3.684704      22.71
 C      -4.085608     2.254983    -4.062635       4.60
 H      -4.025289     1.931729    -5.127192      26.59
 C      -4.192609     0.962566    -1.846507      24.14
 C      -4.301265    -0.280909    -1.079420      89.33
 H      -4.657791    -1.164892    -1.777764      24.22
 O      -5.124453    -0.306258     0.198796     260.43
 H      -4.574234     0.098336     0.941812      25.91
 C      -2.951378    -0.971139    -0.958628      58.43
 H      -2.619062    -0.983039    -1.967558      23.81
 C      -2.882079    -2.403397    -0.332253      99.69
 O      -3.695662    -3.243236    -0.978953     139.19
 H      -3.326826    -3.549037    -2.050961      23.42
 H      -3.040656    -2.565292     0.929503      22.32
 H      -1.680171    -2.609311    -0.326802      23.76
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 C       1.389370     0.024247    -1.479527      35.02
 H       1.694900    -0.301874    -2.455224      26.59
 C       1.441454     0.429031     1.030767      73.86
 H       2.005067     0.412552     1.916142      22.19
 C       0.121322     0.517141     1.028198       9.00
 O      -0.752775     0.951526     2.224645     157.30
 C       0.022380     1.269686     3.483085      98.82
 H       0.936985     1.963010     3.178162      24.97
 H      -0.696696     1.773307     4.270363      24.09
 H       0.273129     0.263074     3.847611      26.50
 C      -0.733580     0.253419    -0.071192      -3.05
 O      -2.138391    -0.079200     0.146903      82.46
 C      -0.046082    -0.007420    -1.352777      33.49
 H      -0.588207    -0.356851    -2.234450      22.23
 C       2.107342     0.156899    -0.226996      19.18
 C       3.627781     0.358518    -0.354232     100.27
 H       3.960235    -0.209741    -1.308999      26.30
 O       3.746218     1.786312    -0.599403     203.92
 H       4.664227     2.059226    -0.237723      21.56
 C       4.569310    -0.155436     0.760581     105.12
 H       4.442690     0.338349     1.777033      25.80
 O       4.585757    -1.544446     1.176333     229.34
 H       4.577260    -1.508792     2.264952      25.92
 C       6.082720     0.181743     0.295317      98.74
 O       6.139887     1.592508     0.537311     127.88
 H       6.761298     1.807612     1.349569      22.58
 H       6.298969    -0.245911    -0.692344      27.83
 H       7.017635    -0.143217     0.876357      28.05
55
name= lig-ACN-Water-frame_895
 C      -4.063163     0.899860    -3.318312      66.14
 H      -4.102880    -0.129850    -3.828960      24.43
 C      -4.037235     2.273820    -1.255338      61.53
 H      -3.976962     2.259187    -0.206810      20.66
 C      -3.924410     3.546177    -1.855142      -2.05
 O      -3.760770     4.688720    -1.213348     243.40
 C      -2.678947     4.790100    -0.436707     129.61
 H      -2.676279     4.157345     0.495134      24.93
 H      -2.821002     5.864428     0.133792      21.06
 H      -1.709181     5.184029    -1.223260      21.77
 C      -4.099264     3.383420    -3.375438     -18.37
 O      -3.971060     4.506605    -4.169578     188.81
 H      -4.060664     5.376206    -3.841491      28.65
 C      -4.032523     2.156146    -3.995353      68.49
 H      -4.089481     2.412563    -5.078907      19.32
 C      -4.139931     0.982241    -1.947577       8.28
 C      -4.391439    -0.422228    -1.009754      81.35
 H      -5.200336    -1.020007    -1.648830      21.98
 O      -5.137050    -0.277430     0.129934     280.43
 H      -4.509049     0.045569     0.889802      24.39
 C      -2.966052    -0.961166    -0.963453      78.38
 H      -2.535434    -0.983111    -1.935609      23.72
 C      -2.791500    -2.273393    -0.306219      89.63
 O      -3.735637    -3.225318    -1.052587     133.85
 H      -3.060541    -3.332683    -1.952344      25.19
 H      -3.386900    -2.038025     0.814328      20.28
 H      -1.736347    -2.747265    -0.421753      22.92
 C       1.293564     0.017235    -1.345503      51.91
 H       1.892731    -0.125676    -2.316879      20.48
 C       1.488295     0.444076     1.040775      61.52
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 H       2.088092     0.899972     1.847410      22.06
 C      -0.017906     0.643590     1.140033      -1.43
 O      -0.640298     0.922914     2.257620     186.80
 C       0.011069     1.214044     3.544644     106.45
 H       0.877536     2.065674     3.707801      23.63
 H      -0.859991     1.670751     4.011315      24.51
 H       0.439448     0.403702     4.111747      26.26
 C      -0.690386     0.201884    -0.138755       3.55
 O      -2.051109    -0.088543    -0.029973     165.14
 C      -0.054584     0.039063    -1.353012      79.60
 H      -0.628188    -0.270336    -2.098187      24.65
 C       2.098497     0.341069    -0.264329      37.37
 C       3.549282     0.372167    -0.423089      86.79
 H       3.859603    -0.151821    -1.424795      24.00
 O       3.732668     1.807653    -0.629642     226.25
 H       4.651932     1.971269    -0.956160      27.14
 C       4.580100    -0.146126     0.712322      87.70
 H       4.203534     0.627822     1.517180      25.02
 O       4.562541    -1.559958     1.149036     257.38
 H       4.706099    -1.527227     2.113877      27.20
 C       6.033546     0.232966     0.298760     102.10
 O       6.288225     1.656213     0.483549     232.51
 H       6.888250     1.742110     1.259470      27.51
 H       6.302003     0.120591    -0.705311      28.68
 H       6.473251    -0.488966     1.027899      27.80
55
name= lig-ACN-Water-frame_896
 C      -4.197440     0.820388    -3.319044      37.57
 H      -4.179777    -0.205276    -3.835481      23.07
 C      -4.006768     2.285755    -1.277418      71.74
 H      -3.811225     2.384056    -0.295954      20.90
 C      -3.948463     3.437016    -2.016338      49.52
 O      -3.851754     4.622089    -1.278468     280.56
 C      -2.612409     4.893627    -0.396706      54.01
 H      -2.185172     3.900008     0.062174      24.48
 H      -2.973239     5.811801     0.279739      20.86
 H      -1.535541     4.980297    -1.133386      21.95
 C      -3.957436     3.349201    -3.309238      22.60
 O      -3.927570     4.429409    -4.140826     185.15
 H      -3.843421     5.320662    -3.576882      26.50
 C      -4.030821     2.048639    -4.008468      28.76
 H      -3.973524     2.045111    -5.103617      19.17
 C      -4.165398     0.966911    -1.857966     -26.16
 C      -4.434313    -0.318139    -1.164871      58.06
 H      -4.957927    -1.175260    -1.896278      22.94
 O      -5.124964    -0.233573     0.161434     243.16
 H      -4.619129     0.416672     0.752436      26.03
 C      -2.783618    -0.907921    -0.932799      79.40
 H      -2.449720    -0.938613    -1.988669      23.33
 C      -2.847302    -2.291570    -0.287925      90.34
 O      -3.702210    -3.219090    -1.110200     225.85
 H      -3.348747    -3.308823    -2.018616      29.57
 H      -3.305473    -2.322011     0.937409      21.79
 H      -1.789665    -2.636925     0.026713      24.70
 C       1.360026     0.057981    -1.382147       9.19
 H       2.007477    -0.102962    -2.386649      17.06
 C       1.391068     0.678547     1.011287      73.33
 H       1.991067     0.914304     1.955059      19.55
 C       0.070295     0.593584     1.053110      18.45
 O      -0.602314     0.903202     2.326967     228.57
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 C      -0.050985     1.215035     3.635074     108.58
 H       0.651739     2.042476     3.195262      23.06
 H      -0.791368     1.511110     4.317464      25.64
 H       0.433383     0.291497     3.957693      26.51
 C      -0.758077     0.166707    -0.015211       2.90
 O      -2.111709    -0.029834    -0.156646     180.69
 C      -0.093974     0.025320    -1.359453      31.89
 H      -0.575116    -0.130343    -2.210524      25.98
 C       2.039908     0.313170    -0.172559      23.95
 C       3.550878     0.265766    -0.490211      62.07
 H       3.752132    -0.267597    -1.541720      20.17
 O       3.814570     1.896134    -0.674706     200.90
 H       4.689839     2.051282    -1.059808      24.41
 C       4.509565    -0.016341     0.679576      95.65
 H       4.415601     0.681996     1.640743      22.21
 O       4.497613    -1.534378     1.049813     276.15
 H       4.441050    -1.680327     1.950337      30.35
 C       5.985871     0.157257     0.333097      92.98
 O       6.488691     1.793564     0.466698     166.84
 H       6.871018     2.012907     1.298233      28.23
 H       6.075854    -0.091511    -0.642578      30.72
 H       6.778646    -0.353857     0.808938      28.28
55
name= lig-ACN-Water-frame_897
 C      -4.274659     0.923104    -3.233832      69.72
 H      -4.605469    -0.004888    -3.758895      22.94
 C      -3.971331     2.110459    -1.156712      45.89
 H      -4.130161     2.106707    -0.126204      23.15
 C      -3.904905     3.306217    -1.929103     -43.84
 O      -3.944250     4.637182    -1.378518     198.87
 C      -2.520852     4.920748    -0.425915      18.51
 H      -2.406064     3.860777     0.067793      21.60
 H      -2.776087     5.536553     0.535749      19.72
 H      -1.695074     5.644483    -1.128695      19.55
 C      -3.838901     3.214019    -3.511863     -20.66
 O      -3.855472     4.457541    -4.177223     184.81
 H      -3.679681     5.163815    -3.435308      18.91
 C      -4.037930     1.976045    -4.097592      84.88
 H      -3.900772     1.746149    -5.125352      27.19
 C      -4.320005     0.945062    -1.902142      49.26
 C      -4.250500    -0.266977    -1.078042      89.95
 H      -4.860451    -1.147154    -1.759966      22.75
 O      -5.080100    -0.198013     0.095114     283.51
 H      -4.674472     0.411280     0.722042      27.51
 C      -2.857768    -0.932278    -0.986282      64.79
 H      -2.199767    -1.128961    -1.880419      22.67
 C      -2.919705    -2.419648    -0.259521      95.75
 O      -3.627868    -3.205972    -1.118885     246.57
 H      -3.142969    -3.276474    -1.840755      34.19
 H      -3.727209    -2.247088     0.766283      20.31
 H      -1.904990    -2.862183    -0.212653      24.57
 C       1.317538     0.109877    -1.391730      54.45
 H       1.635713    -0.232637    -2.510934      22.41
 C       1.443502     0.853713     0.961235      34.01
 H       2.001622     0.949429     1.982694      19.92
 C      -0.060835     0.558747     1.169599     -20.84
 O      -0.761144     0.832286     2.294146     129.45
 C       0.003581     1.225028     3.577210     106.56
 H       0.659850     2.195920     3.905492      23.78
 H      -0.821386     1.404772     4.131655      26.62
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 H       0.632077     0.443002     4.033487      26.30
 C      -0.731108     0.133802    -0.139161      -1.49
 O      -2.218901     0.161769    -0.056926     125.34
 C      -0.002663     0.019117    -1.283329      71.34
 H      -0.647781    -0.093424    -2.111470      22.80
 C       2.134790     0.237308    -0.256627      12.23
 C       3.604952     0.453352    -0.390639      78.90
 H       3.988494    -0.335025    -1.223703      23.33
 O       3.858387     1.836823    -0.696576     242.81
 H       4.812278     1.975765    -0.941141      23.17
 C       4.516533    -0.022276     0.756215      81.63
 H       3.914427     0.397501     1.694572      21.73
 O       4.386833    -1.431216     0.901396     273.33
 H       4.137429    -1.504270     1.926953      25.65
 C       6.108930     0.341641     0.326420     100.64
 O       6.597264     1.743318     0.413867     214.53
 H       6.814660     1.702873     1.425458      26.33
 H       6.289795     0.018517    -0.632786      30.27
 H       6.592870    -0.248476     1.004603      28.54
55
name= lig-ACN-Water-frame_898
 C      -4.416924     0.869570    -3.339889      26.72
 H      -4.696041    -0.114780    -3.699516      27.71
 C      -4.036414     2.154688    -1.148471      70.30
 H      -4.079442     2.263398    -0.010430      20.74
 C      -3.838874     3.275781    -1.981362      14.62
 O      -3.857598     4.595399    -1.437081     226.03
 C      -2.645775     4.920629    -0.501069      72.08
 H      -1.908893     3.955065    -0.429788      25.70
 H      -3.171569     5.490580     0.293685      22.65
 H      -1.982613     5.557017    -1.342861      22.10
 C      -3.789038     3.210309    -3.413162     -34.15
 O      -3.743129     4.445269    -4.201255     178.45
 H      -3.689682     5.145047    -3.587723      28.49
 C      -4.008391     1.980839    -4.215387      33.54
 H      -4.146515     2.099040    -5.273240      15.68
 C      -4.307598     0.940079    -1.811851      -7.41
 C      -4.287947    -0.443673    -1.085468      82.56
 H      -4.958620    -1.303526    -1.719195      22.56
 O      -5.028900    -0.184264     0.071696     302.74
 H      -4.499688     0.163528     0.849262      25.82
 C      -2.890530    -0.951288    -0.775202      69.84
 H      -2.508966    -0.822054    -1.862488      24.11
 C      -2.932531    -2.315376    -0.223843     100.96
 O      -3.644855    -3.304493    -1.204371     183.49
 H      -2.984760    -3.500017    -1.871383      28.83
 H      -3.588996    -2.364689     0.927884      22.50
 H      -2.002852    -2.630165     0.220187      26.75
 C       1.415109     0.047466    -1.404271       4.99
 H       2.126162    -0.089562    -2.374986      18.50
 C       1.362874     0.713701     0.887024      78.09
 H       2.004023     1.355399     1.588598      22.20
 C       0.009737     0.583913     1.077199      20.03
 O      -0.838925     0.801729     2.284593     191.44
 C      -0.066113     1.203916     3.540311      93.68
 H       0.405535     2.213975     2.951822      21.94
 H      -0.752671     1.215330     4.334481      25.84
 H       0.628954     0.351960     3.667924      26.72
 C      -0.839773     0.240499     0.054759       8.76
 O      -2.155917     0.232453     0.011847     136.54
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 C      -0.122593     0.014743    -1.299494      18.81
 H      -0.570696    -0.227943    -2.324235      23.79
 C       2.120728     0.426762    -0.214924      18.73
 C       3.695622     0.499127    -0.333631      87.38
 H       4.002164    -0.079232    -1.335048      24.56
 O       3.897789     1.857126    -0.711215     242.28
 H       4.875497     1.995890    -0.794363      28.65
 C       4.563026     0.090293     0.807946      96.15
 H       4.680758     0.665530     1.832130      24.94
 O       4.286531    -1.366509     0.785796     259.85
 H       4.215353    -1.820104     1.735627      27.26
 C       6.111837     0.378057     0.434803     104.20
 O       6.681418     1.669692     0.443183     224.45
 H       6.839322     2.224593     1.253965      26.94
 H       6.310005     0.046697    -0.569747      28.26
 H       6.704444    -0.190935     1.033121      30.28
55
name= lig-ACN-Water-frame_899
 C      -4.427837     0.850453    -3.411913      56.97
 H      -4.619055    -0.007346    -3.992511      26.68
 C      -4.131314     2.188818    -1.300847      62.11
 H      -3.917441     2.410398    -0.139052      19.31
 C      -3.803583     3.312578    -2.057655      14.30
 O      -3.738132     4.515848    -1.494921     274.74
 C      -2.768738     4.949156    -0.695087     101.29
 H      -2.087172     4.061857    -0.319483      28.25
 H      -3.128594     5.199065     0.298446      25.11
 H      -2.181806     5.972366    -1.040813      22.96
 C      -3.793126     3.262036    -3.434791      40.73
 O      -3.609993     4.343695    -4.166819     191.58
 H      -3.713452     5.155191    -3.620411      27.50
 C      -4.090386     2.027829    -4.043946      59.31
 H      -4.216062     2.063908    -5.132924      19.33
 C      -4.229178     0.857780    -1.920989     -22.69
 C      -4.440143    -0.375677    -1.103983      82.34
 H      -4.706838    -1.358080    -1.779440      22.31
 O      -5.104822    -0.251465     0.189744     250.82
 H      -4.393808     0.254234     0.765654      23.68
 C      -2.878075    -0.823183    -0.724709      81.77
 H      -2.143373    -1.119134    -1.600608      23.88
 C      -2.936540    -2.346510    -0.123647      79.08
 O      -3.592357    -3.318519    -1.163258     113.02
 H      -2.944903    -3.389683    -2.065320      25.69
 H      -3.917761    -2.430422     0.739196      21.24
 H      -1.992420    -2.738093    -0.004090      26.32
 C       1.305686     0.014782    -1.312244      64.08
 H       1.700708    -0.252354    -2.363309      21.12
 C       1.384054     0.693642     1.024168      61.63
 H       1.816715     1.174883     1.928846      22.34
 C      -0.087062     0.627690     1.104291      -2.63
 O      -0.827923     0.750524     2.233957     199.51
 C      -0.129207     1.174497     3.336619     116.33
 H       0.391418     2.406517     3.491715      23.29
 H      -0.764555     1.305811     4.228068      25.45
 H       0.799444     0.640044     3.608107      26.34
 C      -0.726776     0.263342    -0.178545       1.91
 O      -2.227714     0.153297     0.107701     168.69
 C      -0.010561     0.015788    -1.258372      79.29
 H      -0.807562    -0.327997    -2.078885      22.31
 C       2.096761     0.514718    -0.289729      21.05
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 C       3.614038     0.568578    -0.335959      67.00
 H       3.910700    -0.331799    -1.040138      24.08
 O       4.000748     2.062692    -0.750537     164.45
 H       4.937005     2.179283    -0.485597      28.68
 C       4.668627     0.179961     0.862230     100.23
 H       4.118164     0.498479     1.823180      25.03
 O       4.247035    -1.308504     0.756884     270.93
 H       4.567086    -1.624482     1.548374      32.23
 C       6.156850     0.157797     0.542031      93.31
 O       6.760928     1.769105     0.472292     198.15
 H       6.551224     1.952400     1.362023      31.37
 H       6.241165    -0.210542    -0.524401      26.63
 H       6.696381    -0.405816     1.194585      30.16
55
name= lig-ACN-Water-frame_902
 C      -4.444409     0.792618    -3.365506      65.89
 H      -4.580120    -0.164959    -3.936977      24.77
 C      -4.125740     2.307078    -1.300284      26.44
 H      -3.800041     2.366071    -0.184403      17.42
 C      -3.913334     3.372796    -2.174567     -20.87
 O      -3.700097     4.730021    -1.633957     230.86
 C      -2.743347     5.124956    -0.644754     128.72
 H      -1.802197     4.651687    -0.975257      31.35
 H      -3.219860     4.892539     0.371129      25.70
 H      -2.602061     6.126396    -0.771588      24.57
 C      -3.870213     3.151828    -3.695478       2.85
 O      -3.365472     4.270008    -4.358785     156.36
 H      -3.201670     4.830062    -3.611790      24.88
 C      -4.152035     1.916380    -4.246471      70.21
 H      -4.290242     1.842795    -5.339408      19.49
 C      -4.348972     0.865502    -2.000880     -45.59
 C      -4.532099    -0.592799    -1.075977      66.22
 H      -5.252139    -1.379234    -1.484204      22.72
 O      -5.322864    -0.355319     0.167725     240.69
 H      -5.012161     0.257714     0.878655      26.84
 C      -2.957133    -0.902303    -0.718937      89.52
 H      -2.465435    -1.009889    -1.739111      25.01
 C      -2.947926    -2.314109    -0.012511     100.97
 O      -3.424435    -3.353561    -0.947111     219.02
 H      -2.720030    -3.567910    -1.643359      27.01
 H      -3.482518    -2.318980     1.109931      23.29
 H      -1.977201    -2.537598     0.364823      26.80
 C       1.392286     0.213189    -1.368409      30.27
 H       1.726050     0.108371    -2.332623      20.90
 C       1.358379     0.919641     0.964370      86.71
 H       1.784154     1.647750     1.610168      25.02
 C      -0.055326     0.651644     1.007132      10.45
 O      -0.841134     0.683462     2.187768     172.55
 C      -0.273271     1.342845     3.379713      81.91
 H      -0.230591     2.632420     3.073996      21.81
 H      -1.292239     0.963104     3.899563      21.57
 H       0.518480     0.709632     3.758888      26.16
 C      -0.743004     0.073482    -0.059588      19.16
 O      -2.133645    -0.134961     0.106881     162.70
 C       0.023082    -0.107615    -1.279202      55.50
 H      -0.208113    -0.526779    -2.286806      23.28
 C       2.162353     0.756044    -0.176513       7.36
 C       3.748693     0.771485    -0.451739      86.59
 H       4.040638     0.455365    -1.432284      24.51
 O       4.079237     2.325176    -0.553673     201.35
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 H       4.931051     2.280865    -0.085389      27.70
 C       4.542799     0.279612     0.730388      93.74
 H       4.212250     0.786795     1.718582      24.94
 O       4.219376    -1.261089     0.917672     257.76
 H       4.149210    -1.456748     1.886104      28.05
 C       6.063185     0.150560     0.727020      88.66
 O       6.697379     1.692237     0.669030     208.65
 H       7.111430     1.776348     1.504616      30.23
 H       6.423824    -0.514950    -0.177403      26.24
 H       6.354045    -0.281122     1.710493      28.10
55
name= lig-ACN-Water-frame_903
 C      -4.501342     0.873565    -3.294559      46.63
 H      -4.998075    -0.107077    -3.595008      23.80
 C      -4.137687     2.206526    -1.464205      96.90
 H      -4.121084     2.301561    -0.369112      26.03
 C      -3.912310     3.411310    -2.185241      21.69
 O      -3.721765     4.697479    -1.808606     252.32
 C      -2.759736     5.081046    -0.667786     115.14
 H      -1.745501     4.758624    -0.835673      31.99
 H      -3.040164     4.627471     0.388883      26.23
 H      -2.955887     6.064199    -0.654608      24.36
 C      -3.850052     3.181284    -3.546792      -7.46
 O      -3.434293     4.159659    -4.415554     156.15
 H      -3.303187     5.085128    -3.988619      26.76
 C      -4.074589     1.890851    -4.108708      71.23
 H      -3.801541     1.650809    -5.122161      22.43
 C      -4.374742     0.993020    -1.885597       2.67
 C      -4.507235    -0.352522    -1.109475      65.86
 H      -4.782021    -1.145668    -1.862772      24.80
 O      -5.350369    -0.360349     0.076352     255.22
 H      -4.753806     0.282971     0.611554      26.32
 C      -2.960886    -1.085829    -0.783267      59.53
 H      -2.486550    -1.076805    -1.777374      25.63
 C      -2.907109    -2.449614    -0.009417     113.52
 O      -3.372609    -3.445169    -0.841717     255.42
 H      -2.853942    -3.487609    -1.540321      34.66
 H      -3.744023    -2.379684     0.815360      23.29
 H      -1.858469    -2.617097     0.251321      26.49
 C       1.497669     0.298943    -1.459315      60.30
 H       2.163376     0.034006    -2.219158      26.01
 C       1.365222     1.111061     0.896385      57.64
 H       1.844053     1.426224     1.854101      20.27
 C       0.014602     0.606891     1.088052      -2.97
 O      -0.843749     0.697964     2.159898     179.52
 C      -0.424017     1.379900     3.431636      99.48
 H      -0.016430     2.672519     3.362905      22.83
 H      -1.189241     1.477895     4.357401      24.54
 H       0.565712     1.085346     3.806912      26.86
 C      -0.682961    -0.042702    -0.039600      -2.70
 O      -2.096519    -0.034128     0.112116     108.11
 C       0.077799    -0.135472    -1.252072      58.57
 H      -0.561566    -0.591064    -1.986945      23.89
 C       2.117719     0.748963    -0.398678      14.63
 C       3.687546     0.909412    -0.452635      90.31
 H       4.006391     0.287245    -1.251417      27.89
 O       4.045951     2.260558    -0.410294     254.76
 H       4.994731     2.452120    -0.384406      26.35
 C       4.389297     0.164431     0.882985      86.49
 H       4.188298     0.892061     1.700348      25.68
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 O       4.160912    -1.146175     0.927452     322.24
 H       4.029246    -1.470046     1.770570      31.90
 C       6.083436     0.203577     0.755915      75.24
 O       6.692409     1.672421     0.713638     229.72
 H       6.993375     2.064308     1.579541      26.59
 H       6.556489    -0.269260    -0.163495      26.69
 H       6.594668    -0.308866     1.710210      26.28
55
name= lig-ACN-Water-frame_904
 C      -4.542241     0.816927    -3.255855      61.16
 H      -4.787866    -0.089490    -3.905197      23.60
 C      -4.107974     2.311149    -1.258586      59.40
 H      -4.226389     2.535523    -0.263761      27.43
 C      -3.920119     3.360264    -2.146118      -1.15
 O      -3.719280     4.701386    -1.914392     249.51
 C      -2.820632     5.038531    -0.678927      98.84
 H      -1.844438     4.901469    -1.098882      29.85
 H      -3.234766     4.273284     0.130248      22.03
 H      -2.922413     6.036291    -0.448357      21.32
 C      -3.771889     3.154472    -3.591390       6.39
 O      -3.539454     4.128744    -4.490970     197.67
 H      -3.517009     5.100031    -4.097218      23.73
 C      -4.020455     1.901934    -4.044195      42.93
 H      -3.846018     1.860529    -5.098494      22.96
 C      -4.463149     0.979468    -1.867019       3.71
 C      -4.314649    -0.244579    -1.047094      97.04
 H      -4.863621    -0.970358    -1.782637      23.90
 O      -5.308428    -0.330934    -0.045578     263.31
 H      -5.099963    -0.112379     0.891065      27.81
 C      -2.948067    -1.048832    -0.792955      73.30
 H      -2.476190    -1.385433    -1.696574      25.45
 C      -2.892470    -2.398330    -0.012793      98.82
 O      -3.349856    -3.640257    -0.826115     150.84
 H      -2.950361    -3.588616    -1.803562      27.78
 H      -3.512790    -2.416230     0.951429      24.87
 H      -1.921797    -2.563241     0.437492      26.28
 C       1.397304     0.191099    -1.524465      21.96
 H       1.690718    -0.101806    -2.563938      22.96
 C       1.370915     1.141527     0.816254      53.29
 H       2.070210     1.524917     1.656810      21.00
 C       0.099241     0.585071     1.058350       6.34
 O      -0.821754     0.778602     2.263288     144.88
 C      -0.441721     1.470618     3.448509      84.95
 H      -0.380611     2.664094     2.898067      20.62
 H      -1.430430     1.331216     4.104275      23.62
 H       0.404094     0.910580     3.941657      24.73
 C      -0.553545     0.034156    -0.073593      -1.36
 O      -2.062964    -0.052933     0.030013      90.12
 C       0.072271    -0.196364    -1.301742      53.55
 H      -0.409365    -0.503077    -2.163699      22.34
 C       2.126665     0.874100    -0.322403      -7.49
 C       3.620606     0.890753    -0.248408     103.40
 H       3.973412     0.532784    -1.171829      25.47
 O       4.055258     2.308870    -0.329450     228.42
 H       5.035233     2.113242    -0.442507      25.15
 C       4.476403     0.295806     0.909362      95.85
 H       4.034932     0.529283     1.837585      24.98
 O       3.998073    -1.200694     0.930312     233.09
 H       4.361419    -1.484474     1.906841      26.27
 C       6.046311     0.442561     0.826992      95.97
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 O       6.663538     1.604746     0.724127     290.94
 H       6.666518     1.990608     1.700960      25.77
 H       6.166050    -0.090168    -0.152163      26.62
 H       6.458053    -0.371295     1.617031      26.46
55
name= lig-ACN-Water-frame_905
 C      -4.426306     0.842578    -3.251318      55.76
 H      -4.527392    -0.248422    -3.458654      24.34
 C      -4.172116     2.344647    -1.140797      71.86
 H      -3.992980     2.330835    -0.155756      16.99
 C      -3.865409     3.392944    -2.154549     -12.87
 O      -3.706098     4.772363    -1.895705     269.70
 C      -2.915163     4.987223    -0.767077     102.81
 H      -1.868456     4.832594    -0.997412      29.78
 H      -2.994740     4.214771     0.153243      25.84
 H      -3.223221     5.921480    -0.318630      22.26
 C      -3.749444     3.078401    -3.585548      -7.18
 O      -3.631320     4.179718    -4.548594     171.15
 H      -3.651002     4.912030    -3.915721      26.14
 C      -4.056085     1.813032    -4.162745      57.24
 H      -4.271256     1.644194    -5.188382      22.42
 C      -4.355494     1.085530    -1.816713     -23.82
 C      -4.259907    -0.440795    -1.043199      62.25
 H      -4.513768    -1.351383    -1.728894      25.28
 O      -5.322970    -0.295312    -0.010832     243.39
 H      -4.877089    -0.242582     0.838893      27.81
 C      -2.809423    -0.901959    -0.775286      93.31
 H      -2.505638    -0.871549    -1.779239      25.83
 C      -2.957170    -2.416204    -0.030877      95.16
 O      -3.297289    -3.705090    -0.785915     114.67
 H      -2.560829    -3.626111    -1.712072      23.15
 H      -3.677538    -2.364689     0.722713      25.88
 H      -1.871567    -2.549297     0.211794      24.53
 C       1.397625     0.131022    -1.406131      57.04
 H       2.101583     0.219488    -2.331135      16.34
 C       1.382448     1.083096     0.899552      37.97
 H       1.782765     1.867416     1.686156      19.99
 C       0.003855     0.689072     1.075831      15.05
 O      -0.731980     0.750617     2.180868     194.21
 C      -0.453318     1.579486     3.392803     108.02
 H      -0.185077     2.851969     3.578952      21.48
 H      -1.411130     1.471305     3.981396      24.23
 H       0.395826     1.275925     4.074630      24.69
 C      -0.695509     0.107042    -0.108345      10.36
 O      -1.946540    -0.128084    -0.063008     175.21
 C       0.045422    -0.209318    -1.370481      66.02
 H      -0.490852    -0.628744    -2.155794      23.22
 C       2.052900     0.793137    -0.393394      -7.83
 C       3.654006     0.923144    -0.212056      79.68
 H       4.016312     0.278716    -0.966056      24.51
 O       4.095632     2.400273    -0.285047     224.18
 H       5.050665     2.646867    -0.228571      22.92
 C       4.346152     0.321856     1.058913      85.65
 H       4.233572     0.947532     1.871472      24.15
 O       3.925718    -1.191136     0.960159     217.03
 H       4.602170    -1.854370     1.482795      25.47
 C       5.859751     0.323578     0.770777      92.98
 O       6.683524     1.714488     0.774374     289.82
 H       6.764754     2.237656     1.605028      30.08
 H       6.240664    -0.109212    -0.142784      26.63
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 H       6.398199    -0.153248     1.748786      24.56
55
name= lig-ACN-Water-frame_906
 C      -4.227875     0.814844    -3.142559      36.53
 H      -4.592028    -0.118211    -3.566114      23.03
 C      -4.133365     2.304784    -1.315912      74.86
 H      -4.122769     2.558865    -0.297169      20.26
 C      -3.833933     3.362675    -2.220699     -10.41
 O      -3.751533     4.744675    -1.906878     232.03
 C      -2.895373     5.003015    -0.688823     103.29
 H      -1.838864     5.142690    -0.977151      28.32
 H      -3.254384     4.180089     0.043338      23.82
 H      -3.183799     6.029841    -0.362092      22.00
 C      -3.840922     3.098934    -3.642518      -2.88
 O      -3.708858     4.183951    -4.455325     187.32
 H      -3.517767     5.112146    -4.238685      23.60
 C      -4.151859     1.791527    -4.205752      69.43
 H      -4.153596     1.645147    -5.286789      27.55
 C      -4.182167     0.939075    -1.741620      27.77
 C      -4.328336    -0.346121    -1.076425      80.76
 H      -4.777800    -1.002480    -1.879100      24.64
 O      -5.277125    -0.343631     0.077025     215.10
 H      -4.721463     0.177772     0.798599      26.05
 C      -2.809172    -0.981851    -0.868495      87.40
 H      -2.363962    -1.185864    -1.788868      26.42
 C      -2.873414    -2.432486    -0.130551     113.79
 O      -3.216491    -3.611692    -0.779159     213.85
 H      -2.452441    -4.041096    -1.431161      25.13
 H      -3.589753    -2.325239     0.613440      26.89
 H      -2.063866    -2.588904     0.605233      26.57
 C       1.503685     0.143797    -1.360584      22.82
 H       2.032256    -0.391391    -2.323158      20.73
 C       1.306399     1.044105     0.925576      63.82
 H       1.835612     1.539031     1.851077      21.07
 C      -0.035705     0.791376     0.894618       7.97
 O      -0.716573     0.783685     2.180647     180.20
 C      -0.457921     1.669876     3.405001      81.40
 H      -0.300380     2.633003     2.599195      21.90
 H      -1.322923     1.619039     4.039813      25.06
 H       0.448238     1.121674     3.797703      24.05
 C      -0.593282     0.147742    -0.233087      21.16
 O      -2.032959    -0.118622     0.068105     167.72
 C       0.046336    -0.157154    -1.327945      60.89
 H      -0.420529    -0.774779    -2.102640      21.54
 C       2.142360     0.753012    -0.174253      -0.54
 C       3.650910     1.027197    -0.276795      98.63
 H       4.162750     0.615475    -1.111591      23.53
 O       4.046509     2.408192    -0.295512     248.38
 H       4.875279     2.235484     0.169880      25.90
 C       4.226099     0.270623     1.080403     108.28
 H       3.837324     0.520619     2.004779      26.09
 O       3.889682    -1.054743     1.046379     311.94
 H       4.593598    -1.524086     1.422563      29.77
 C       5.867044     0.309259     0.842913      72.79
 O       6.606840     1.771728     0.761931     231.18
 H       6.881826     1.797547     1.662373      28.50
 H       6.027575    -0.148030    -0.106989      28.67
 H       6.347612    -0.453876     1.702659      26.83
55
name= lig-ACN-Water-frame_907
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 C      -4.113289     0.710786    -3.264913      61.79
 H      -4.247083    -0.266359    -3.648883      21.72
 C      -3.989696     2.275666    -1.402867      56.24
 H      -4.391295     2.548862    -0.410231      21.61
 C      -3.874028     3.317770    -2.328449      -6.03
 O      -3.768036     4.650384    -1.889607     209.42
 C      -2.927100     5.075716    -0.635813      80.52
 H      -1.853418     4.915964    -0.969987      26.27
 H      -2.925631     4.402144     0.285064      24.98
 H      -3.329866     6.099152    -0.250413      21.84
 C      -3.973183     3.148299    -3.656149      44.08
 O      -3.739272     4.226120    -4.498151     166.85
 H      -3.552644     4.755584    -3.597817      18.23
 C      -4.146136     1.876548    -4.022846      51.33
 H      -4.188099     1.606958    -5.100748      26.37
 C      -4.061131     0.963991    -1.877512      -4.97
 C      -4.360961    -0.353779    -1.028762      77.10
 H      -5.037732    -0.926113    -1.656669      24.81
 O      -5.101350    -0.383014     0.181811     247.01
 H      -5.000066     0.401122     0.828268      24.61
 C      -2.881738    -1.150457    -0.884579      60.72
 H      -2.401275    -1.072420    -1.820477      24.98
 C      -2.834273    -2.345099    -0.040362     114.27
 O      -3.152027    -3.600196    -0.851665     240.19
 H      -2.453356    -3.763986    -1.373523      31.74
 H      -3.618889    -2.212594     0.570642      26.97
 H      -1.787537    -2.369933     0.418142      25.51
 C       1.546041     0.119859    -1.270981      40.37
 H       2.351669    -0.331608    -2.107487      21.54
 C       1.372360     1.091422     0.926424      46.60
 H       1.785259     1.213749     1.969985      18.84
 C      -0.061597     0.855258     0.956973       6.76
 O      -0.833108     0.778310     2.136022     203.16
 C      -0.378421     1.702165     3.171231     119.81
 H      -0.193776     2.990564     3.089986      24.55
 H      -1.229548     1.733135     3.764710      26.85
 H       0.486208     1.593107     3.873640      26.39
 C      -0.802264     0.217747    -0.134188     -11.73
 O      -2.095686    -0.113966     0.119394      35.97
 C       0.241315    -0.142644    -1.380410      52.87
 H      -0.056719    -0.690728    -2.346565      23.17
 C       2.174709     0.717744    -0.195852      42.33
 C       3.615446     0.979312    -0.201606     101.59
 H       3.797710     0.485835    -1.124740      25.54
 O       3.994860     2.406539    -0.277304     233.01
 H       4.710525     2.756242     0.252324      26.66
 C       4.313115     0.393645     1.005490     104.64
 H       4.014165     1.121471     1.723710      27.31
 O       3.840125    -1.058738     1.082038     293.72
 H       4.267724    -1.508365     1.818454      29.73
 C       5.859289     0.410609     0.926852     104.53
 O       6.438374     1.638828     0.788187     306.29
 H       6.986782     2.093428     1.469685      28.84
 H       6.024151    -0.063080    -0.025859      28.45
 H       6.570048    -0.220929     1.724979      25.72
55
name= lig-ACN-Water-frame_908
 C      -4.024124     0.647998    -3.335927      60.65
 H      -3.891488    -0.300212    -3.775479      24.36
 C      -3.935674     2.198962    -1.396972      85.63
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 H      -3.792468     2.257955    -0.232456      22.64
 C      -3.888141     3.376785    -2.175159      -0.40
 O      -3.761309     4.640148    -1.782430     223.88
 C      -2.967361     5.046359    -0.665673     121.15
 H      -1.839800     5.260066    -0.980386      26.13
 H      -3.259814     4.422004     0.165362      27.72
 H      -3.358096     6.184743    -0.626842      22.31
 C      -4.039690     3.187107    -3.665219     -54.98
 O      -3.757183     4.315541    -4.505564     154.49
 H      -3.602205     5.246197    -4.290135      27.54
 C      -4.115363     1.784447    -4.215856       6.40
 H      -4.278916     1.802630    -5.327708      17.02
 C      -4.053736     0.892293    -1.921120      31.83
 C      -4.262476    -0.463394    -1.021503      87.52
 H      -4.780807    -1.203772    -1.633119      26.68
 O      -4.969187    -0.374784     0.303003     279.93
 H      -4.465637     0.293288     0.768241      27.57
 C      -2.952323    -1.004166    -0.822483      91.92
 H      -2.423171    -1.266233    -1.755413      27.26
 C      -2.887422    -2.414177     0.011384     104.18
 O      -3.070818    -3.565372    -0.872219     249.66
 H      -2.589103    -3.365971    -1.612220      32.23
 H      -3.298057    -2.507402     0.894513      28.97
 H      -1.710760    -2.554772     0.249615      25.78
 C       1.620686     0.070336    -1.247039       0.03
 H       2.313035    -0.000654    -2.262092      18.01
 C       1.296591     1.084281     0.984807      71.94
 H       1.847200     1.611870     1.740238      22.78
 C      -0.080318     0.761877     0.983291      14.87
 O      -0.852059     0.877955     2.088410     175.10
 C      -0.399473     1.804361     3.098740      87.74
 H      -0.276864     2.805705     2.288345      22.33
 H      -1.057671     1.807719     3.907976      26.58
 H       0.529915     1.264304     3.324972      25.82
 C      -0.694101     0.236586    -0.237765      20.99
 O      -2.148767    -0.134857     0.025260      72.33
 C       0.081270    -0.124133    -1.233798      42.16
 H      -0.424330    -0.581830    -2.189971      25.12
 C       2.112693     0.812417    -0.110467     -16.70
 C       3.694819     0.906235    -0.202064      98.49
 H       4.313733     0.459357    -0.939713      23.35
 O       3.876581     2.450153    -0.311371     188.74
 H       4.766190     2.423657     0.193406      21.70
 C       4.393708     0.434562     1.051287      96.62
 H       4.204525     0.944663     1.987260      23.21
 O       3.824690    -0.990564     1.139275     258.25
 H       4.032406    -1.387348     2.126354      26.89
 C       5.887768     0.300791     0.908885      84.73
 O       6.352646     1.729588     0.782644     335.18
 H       6.655472     1.781037     1.760055      25.60
 H       6.337844    -0.384063     0.224410      26.82
 H       6.009816    -0.140216     2.086573      23.90
55
name= lig-ACN-Water-frame_909
 C      -3.991408     0.726274    -3.435181      25.97
 H      -4.105663    -0.270491    -3.836261      22.80
 C      -3.900574     2.083779    -1.344409      25.71
 H      -3.408684     2.232207    -0.258706      16.85
 C      -3.915777     3.268076    -2.185104      -4.03
 O      -3.802042     4.680649    -1.755490     238.70
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 C      -2.996394     5.117366    -0.648332      95.27
 H      -1.841203     4.839726    -0.848326      26.21
 H      -3.159224     4.608639     0.297684      27.56
 H      -3.294672     6.230847    -0.257302      22.15
 C      -3.979681     3.203131    -3.628653     -11.60
 O      -3.802226     4.263118    -4.544035     191.60
 H      -3.995384     4.996096    -3.953211      22.74
 C      -4.054082     1.903660    -4.340332      38.57
 H      -3.955524     1.637724    -5.425567      27.06
 C      -4.116546     0.749253    -1.946905      10.68
 C      -4.230580    -0.445923    -1.034861      90.39
 H      -4.906213    -1.214887    -1.460822      24.32
 O      -4.873380    -0.340457     0.294027     276.19
 H      -4.469326     0.162922     0.991129      26.45
 C      -2.806415    -1.111339    -0.668379      77.51
 H      -2.403889    -1.246212    -1.700090      23.02
 C      -2.765905    -2.497046    -0.011717     108.02
 O      -3.080803    -3.532302    -0.893096     222.89
 H      -2.620046    -3.512310    -1.890000      24.75
 H      -3.484905    -2.566884     0.661688      26.83
 H      -1.650055    -2.432572     0.466325      24.54
 C       1.397276     0.122134    -1.225473      61.54
 H       1.891339    -0.261611    -2.231753      23.35
 C       1.277792     1.115780     0.988902      37.79
 H       1.447351     1.778975     1.759497      23.51
 C      -0.067633     0.679711     0.987303      19.79
 O      -0.959742     0.950388     2.039169     189.34
 C      -0.354502     1.874420     2.995794     108.23
 H      -0.179461     3.129314     2.688895      22.79
 H      -1.096612     2.028311     3.796333      25.09
 H       0.595219     1.723723     3.475350      25.76
 C      -0.730693     0.165081    -0.102280       1.08
 O      -2.051593    -0.024313    -0.073050     147.89
 C       0.126513    -0.156927    -1.307926      57.44
 H      -0.466688    -0.635718    -2.172301      21.90
 C       2.157206     0.716538    -0.167069     -13.00
 C       3.652789     1.054057    -0.167429     102.71
 H       3.828791     0.518705    -1.090114      22.32
 O       3.828406     2.401525    -0.351162     254.89
 H       4.755025     2.771728    -0.281418      24.43
 C       4.372184     0.288065     1.120597      98.64
 H       4.119146     0.968507     1.990891      22.19
 O       3.803527    -0.906765     1.238114     284.75
 H       4.184001    -1.284859     2.091686      27.53
 C       5.920672     0.199350     1.017527      74.22
 O       6.323063     1.803988     0.805888     272.89
 H       6.985072     2.121973     1.484913      28.32
 H       6.221274    -0.447434     0.139201      25.00
 H       6.650192    -0.053222     1.995255      23.75
55
name= lig-ACN-Water-frame_910
 C      -4.123121     0.780232    -3.443716      78.31
 H      -4.298806    -0.096589    -4.100887      23.25
 C      -3.862475     2.043556    -1.447895      50.61
 H      -3.978556     2.117439    -0.266172      23.92
 C      -3.893350     3.211970    -2.233815     -11.95
 O      -3.904483     4.628866    -1.801763     207.93
 C      -2.971465     5.103100    -0.499844      86.14
 H      -1.865119     4.975337    -0.963442      24.03
 H      -3.380255     4.510931     0.277127      25.20
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 H      -3.081486     6.323958    -0.642372      22.46
 C      -3.879141     3.128940    -3.672621      14.80
 O      -3.887878     4.213378    -4.461858     195.64
 H      -3.961414     5.095612    -3.942656      23.18
 C      -3.911970     1.902537    -4.181175      65.13
 H      -3.757289     2.051644    -5.261320      23.62
 C      -4.084047     0.841838    -2.053717      14.29
 C      -4.164160    -0.547302    -0.956301      75.20
 H      -4.684404    -1.273240    -1.617806      24.04
 O      -4.878778    -0.277554     0.234793     256.89
 H      -4.214669     0.280849     0.643182      26.56
 C      -2.672425    -1.184541    -0.812423      73.17
 H      -2.046801    -1.351715    -1.738781      22.95
 C      -2.659970    -2.489937     0.061095      97.72
 O      -3.126878    -3.558678    -0.974704     140.24
 H      -2.121965    -3.675965    -1.597716      22.14
 H      -3.368651    -2.359890     0.751687      27.06
 H      -1.784205    -3.093909     0.655823      23.17
 C       1.447970     0.162167    -1.280094      29.92
 H       2.194300    -0.162273    -2.042625      23.09
 C       1.289891     1.109606     0.898613      73.77
 H       1.946198     1.561232     1.592524      19.06
 C      -0.065946     0.698992     1.013301      -0.49
 O      -0.953358     1.070272     2.052410     172.23
 C      -0.406530     2.040998     3.033937      87.75
 H      -0.395154     3.095399     2.343882      22.80
 H      -1.186107     1.942936     3.839842      25.26
 H       0.476865     1.558086     3.404349      25.70
 C      -0.649574    -0.029302    -0.139268      11.48
 O      -2.051832     0.092043    -0.069003     155.16
 C      -0.042109    -0.205035    -1.292736      59.32
 H      -0.218017    -0.669930    -2.233119      21.16
 C       2.027614     0.683391    -0.125474      29.27
 C       3.563638     0.950755    -0.184310      73.38
 H       4.167089     0.501858    -0.965249      24.05
 O       3.817593     2.469752    -0.388138     222.50
 H       4.754968     2.395294    -0.522846      26.82
 C       4.416866     0.423924     1.157124      67.99
 H       4.140203     1.166744     2.002230      22.26
 O       3.720684    -1.022321     1.380367     304.99
 H       4.309638    -1.599268     1.765341      30.65
 C       5.974319     0.395807     1.054053      83.55
 O       6.307454     1.739919     0.788008     326.76
 H       7.102006     1.742330     1.307684      28.61
 H       6.249883    -0.069636     0.026003      25.20
 H       6.552409    -0.288936     1.897759      24.41
55
name= lig-ACN-Water-frame_911
 C      -4.220657     0.640388    -3.451993      19.50
 H      -4.409888    -0.433217    -3.843106      24.33
 C      -3.927277     2.136467    -1.498381      52.94
 H      -4.162568     2.272325    -0.395632      23.80
 C      -3.796761     3.350197    -2.190010      36.41
 O      -3.959751     4.558590    -1.742428     256.83
 C      -3.036621     5.001782    -0.620289      89.75
 H      -1.901196     4.615443    -0.578325      26.69
 H      -3.317373     4.806325     0.438920      25.84
 H      -3.340390     6.236674    -0.505232      22.76
 C      -3.775017     3.165948    -3.554934       7.06
 O      -3.968772     4.265683    -4.410410     163.96
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 H      -3.620288     5.056522    -3.892608      25.58
 C      -3.789286     1.833071    -4.237364      30.55
 H      -3.917261     1.620081    -5.289913      18.08
 C      -4.024659     0.706688    -2.012099     -12.91
 C      -4.052657    -0.610208    -1.192713      72.65
 H      -4.761586    -1.464274    -1.447215      23.38
 O      -4.834947    -0.219263     0.139996     168.89
 H      -4.379670     0.281359     0.867736      26.96
 C      -2.620744    -1.046937    -0.817423      86.48
 H      -2.270155    -1.272686    -1.892391      26.77
 C      -2.695489    -2.557588     0.004065      95.84
 O      -3.139268    -3.537694    -0.937161     170.92
 H      -2.291009    -3.838921    -1.594818      23.94
 H      -3.358999    -2.548274     0.842977      27.49
 H      -1.530994    -2.634143     0.332923      25.22
 C       1.461066     0.062365    -1.398577      64.42
 H       1.927751     0.031634    -2.326558      24.13
 C       1.279237     1.084642     0.994145      43.97
 H       1.597421     1.593370     1.941451      20.58
 C      -0.073764     0.768953     0.999946      20.34
 O      -0.874408     1.168134     2.041422     229.31
 C      -0.503614     2.122955     3.038617     125.46
 H      -0.231584     3.191126     2.661401      25.79
 H      -1.230943     2.371585     3.938461      24.30
 H       0.435921     1.904610     3.499754      26.84
 C      -0.665028     0.037259    -0.050338     -32.17
 O      -2.079325    -0.035009    -0.105723     132.85
 C       0.168104    -0.257694    -1.353210      48.87
 H      -0.515622    -0.523914    -2.000827      26.44
 C       2.078178     0.696028    -0.233669       1.50
 C       3.579654     0.834837    -0.126535      82.69
 H       3.900958     0.253269    -1.038293      22.26
 O       3.836340     2.406667    -0.433643     163.74
 H       4.845586     2.607823    -0.448449      23.39
 C       4.279176     0.441549     1.153722      82.94
 H       4.057026     0.845020     2.235310      19.66
 O       3.737449    -1.014022     1.518554     276.62
 H       4.567128    -1.599735     1.413024      26.96
 C       5.825722     0.434647     0.894562      98.05
 O       6.416771     1.762583     0.783441     323.51
 H       7.012477     2.022567     1.558240      31.16
 H       6.198230    -0.467243     0.246734      27.01
 H       6.153176     0.153324     1.999430      23.94
55
name= lig-ACN-Water-frame_912
 C      -4.073834     0.604947    -3.415231      74.30
 H      -4.402533    -0.322689    -4.027219      23.15
 C      -4.002057     2.037485    -1.388664      56.52
 H      -3.916993     2.156430    -0.336285      20.89
 C      -3.742624     3.182709    -2.208580     -56.13
 O      -3.991948     4.606289    -1.611626     172.62
 C      -3.146610     4.972256    -0.607276      97.05
 H      -2.113821     4.536422    -1.012523      26.87
 H      -3.600522     4.503723     0.329525      23.01
 H      -2.760606     6.188450    -0.787074      20.74
 C      -3.708927     3.058980    -3.726909     -14.06
 O      -3.982616     4.314879    -4.371667     150.79
 H      -3.587043     4.981027    -3.836073      25.27
 C      -3.868236     1.750824    -4.199319      61.02
 H      -3.901062     1.843510    -5.255270      23.30
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 C      -4.043895     0.738122    -2.069777      31.52
 C      -4.084719    -0.458278    -1.167157      97.90
 H      -4.446702    -1.235617    -1.970138      25.39
 O      -4.801768    -0.238485    -0.007723     242.91
 H      -4.069672     0.339767     0.459130      24.32
 C      -2.767395    -1.159170    -0.858516      94.69
 H      -2.038247    -1.307984    -1.702695      25.96
 C      -2.676274    -2.423223    -0.178241     114.74
 O      -3.165206    -3.580454    -0.872244     234.59
 H      -2.706088    -3.551565    -1.678886      32.24
 H      -3.211544    -2.503816     0.759186      26.97
 H      -1.532897    -2.652832     0.175776      25.55
 C       1.553182     0.088427    -1.405483      34.28
 H       2.020738     0.006076    -2.284643      22.54
 C       1.343043     0.979883     0.901934      56.33
 H       1.952701     1.563187     1.714934      19.34
 C      -0.069639     0.861291     0.979342       9.49
 O      -0.900151     1.233677     2.057454     157.78
 C      -0.480696     2.294647     3.079246      97.91
 H      -0.552370     3.220054     2.548188      25.78
 H      -1.477922     1.958346     3.551742      21.48
 H       0.299053     1.976804     3.771692      25.47
 C      -0.640407     0.159854    -0.170956      14.29
 O      -1.962428    -0.140663    -0.057963     146.12
 C       0.095167    -0.268059    -1.196051      63.54
 H      -0.173875    -0.588959    -2.061506      26.68
 C       2.089370     0.711590    -0.209352      15.81
 C       3.556021     0.900752    -0.170839     114.23
 H       4.118681     0.209400    -0.894453      21.38
 O       3.878655     2.210435    -0.491585     236.73
 H       4.728818     2.505918     0.033935      21.72
 C       4.144496     0.320407     1.145717     108.66
 H       3.810634     1.270878     1.742039      21.61
 O       3.853216    -0.916641     1.604885     284.35
 H       4.565761    -1.672542     1.297516      24.73
 C       5.676263     0.383435     1.007941      76.22
 O       6.502175     1.823435     0.692607     264.83
 H       6.964823     1.659372     1.619484      25.77
 H       5.987498    -0.133748    -0.028868      23.27
 H       6.194869    -0.106173     1.904652      24.60
55
name= lig-ACN-Water-frame_913
 C      -3.903328     0.676548    -3.487570      18.23
 H      -4.007290    -0.409255    -3.884461      22.60
 C      -3.927040     2.027123    -1.384404      64.99
 H      -4.062335     2.051145    -0.388615      23.72
 C      -3.849727     3.134198    -2.228230      15.61
 O      -4.104560     4.452344    -1.765590     162.12
 C      -3.015732     4.939202    -0.525055      57.13
 H      -2.025465     4.332515    -0.495606      25.08
 H      -3.354834     4.923905     0.636673      22.15
 H      -3.107414     6.239638    -0.520041      22.70
 C      -3.787580     3.079296    -3.584312      16.24
 O      -3.909476     4.231214    -4.349186     161.46
 H      -3.914440     4.946203    -3.631895      17.69
 C      -3.954065     1.812210    -4.328469      42.23
 H      -4.043605     1.560264    -5.348137      33.61
 C      -4.028658     0.802809    -2.037169      29.81
 C      -4.121976    -0.469095    -1.282872      91.02
 H      -4.990176    -1.185194    -1.670847      23.50
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 O      -4.824119    -0.263779    -0.042336     259.11
 H      -4.448577     0.221668     0.739155      25.57
 C      -2.692446    -1.096373    -1.049328      59.48
 H      -2.406750    -1.202920    -2.120291      25.38
 C      -2.656004    -2.446158    -0.125159      95.63
 O      -3.236110    -3.632812    -0.882584     230.63
 H      -2.784010    -3.745795    -1.655011      33.20
 H      -3.139119    -2.082015     0.852368      23.95
 H      -1.501856    -2.625143    -0.072660      24.83
 C       1.444431     0.135064    -1.317919      64.85
 H       2.090229    -0.258092    -1.990223      26.02
 C       1.349476     1.015636     0.880969      53.64
 H       1.923463     1.384698     1.850486      21.07
 C      -0.021037     0.930566     0.927381      16.98
 O      -0.848792     1.267342     1.998817     206.94
 C      -0.623631     2.345431     3.078717     102.62
 H      -0.453933     3.275314     2.676042      27.46
 H      -1.340465     2.653273     3.941909      23.76
 H       0.366087     2.020053     3.461628      24.40
 C      -0.655371     0.246139    -0.175868     -37.20
 O      -1.966262    -0.202849     0.076026      61.88
 C       0.184141    -0.235668    -1.314175      68.16
 H      -0.289783    -0.947515    -1.808911      27.16
 C       2.132473     0.661688    -0.245402      29.87
 C       3.576964     0.732101    -0.326513      82.40
 H       3.937877     0.129142    -1.249242      22.72
 O       3.966493     2.166975    -0.500786     202.73
 H       4.768927     2.354788     0.039393      22.58
 C       4.202675     0.514131     1.161517      96.15
 H       3.798771     0.915321     2.126166      21.94
 O       3.888949    -0.911613     1.698018     296.47
 H       4.555304    -1.485126     1.333691      28.52
 C       5.746159     0.462549     1.019847      82.31
 O       6.458949     1.697793     0.703447     316.62
 H       7.149107     2.122535     1.279196      30.99
 H       5.822475    -0.194475    -0.023703      24.66
 H       6.190984    -0.170754     1.748898      27.66
55
name= lig-ACN-Water-frame_914
 C      -3.820963     0.730856    -3.506709      70.00
 H      -3.647725    -0.255716    -4.030395      23.83
 C      -3.891051     2.033396    -1.401427      61.94
 H      -4.091748     2.235146    -0.409519      23.42
 C      -3.980255     3.144071    -2.178983     -11.38
 O      -4.068841     4.416457    -1.727511     237.06
 C      -3.017495     4.933101    -0.471114      47.75
 H      -2.045623     4.415864    -0.748835      24.09
 H      -3.860714     4.516619     0.240112      17.18
 H      -2.862643     5.982756    -1.179763      19.15
 C      -3.984649     3.016014    -3.667492     -17.97
 O      -3.813061     4.187853    -4.314434     159.53
 H      -4.247445     4.954450    -3.783035      22.98
 C      -3.938771     1.870378    -4.341150      96.78
 H      -3.980074     2.045268    -5.398060      26.28
 C      -3.935030     0.764901    -2.134368      30.02
 C      -4.136873    -0.525766    -1.256995      73.61
 H      -4.547746    -1.394692    -1.986358      22.30
 O      -4.940538    -0.301202     0.044968     238.84
 H      -4.215954     0.046419     0.567672      24.65
 C      -2.673302    -1.064869    -1.047826      68.90
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 H      -1.917380    -0.924020    -1.778209      22.66
 C      -2.624978    -2.484223    -0.281075      90.98
 O      -3.329730    -3.606142    -0.815208     229.13
 H      -2.508109    -4.021624    -1.391803      25.25
 H      -3.340721    -2.472080     0.670094      21.27
 H      -1.611560    -2.757521     0.179088      24.57
 C       1.481079     0.071459    -1.419378      16.46
 H       1.972539    -0.345632    -2.294484      20.60
 C       1.396366     1.156450     0.962017      58.24
 H       1.771683     1.482693     2.010413      17.81
 C      -0.029081     1.013078     0.865297       3.91
 O      -0.888239     1.309557     1.986791     186.36
 C      -0.581381     2.381476     2.958614      99.51
 H      -0.546835     3.238831     2.413675      26.71
 H      -1.556927     2.105581     3.525733      21.51
 H       0.313301     2.242425     3.712648      23.09
 C      -0.699941     0.218898    -0.179665      12.22
 O      -1.993655    -0.246636     0.042719     173.27
 C      -0.038496    -0.198039    -1.310895      53.62
 H      -0.244808    -0.943522    -2.044384      20.97
 C       2.130738     0.665657    -0.219431      12.76
 C       3.674834     0.687276    -0.210863      85.90
 H       4.140255    -0.112394    -0.930947      21.57
 O       4.041382     2.209402    -0.550057     178.12
 H       5.026332     2.281725    -0.462131      24.35
 C       4.320962     0.451954     1.153630      98.69
 H       3.948478     1.418507     1.517773      24.32
 O       3.916241    -0.866770     1.733842     322.77
 H       4.577776    -1.500052     1.522715      28.68
 C       5.858179     0.426635     0.989930     110.38
 O       6.435200     1.674276     0.678242     312.41
 H       6.705195     1.708800     1.598687      27.59
 H       6.234924    -0.429804     0.203970      25.88
 H       6.247365     0.187845     1.919571      26.71
55
name= lig-ACN-Water-frame_915
 C      -3.781571     0.647597    -3.606926      44.20
 H      -3.751899    -0.311009    -4.137481      22.02
 C      -3.974040     1.939024    -1.434750      63.56
 H      -3.800846     1.821784    -0.353028      17.03
 C      -4.059258     3.134572    -2.248769      -9.63
 O      -4.004527     4.525680    -1.631467     252.82
 C      -3.135185     4.853398    -0.706464      95.26
 H      -2.296589     4.180976    -0.446508      28.39
 H      -3.406271     5.027576     0.544414      20.67
 H      -2.835694     6.076926    -0.427746      21.41
 C      -4.124176     3.129031    -3.610245     -13.54
 O      -3.794901     4.254636    -4.367829     166.90
 H      -3.960534     5.024900    -3.806559      26.13
 C      -3.881897     1.844895    -4.320526       4.73
 H      -3.578236     1.780473    -5.383016      22.12
 C      -3.878852     0.714644    -2.084753      -9.33
 C      -4.044457    -0.545274    -1.210602      79.16
 H      -4.698972    -1.351588    -1.807198      23.58
 O      -4.935875    -0.382272    -0.021147     208.63
 H      -4.477914     0.060871     0.796845      25.08
 C      -2.646510    -1.121652    -0.851385     116.95
 H      -2.416088    -1.209202    -1.883167      24.66
 C      -2.698985    -2.485991    -0.290893     108.52
 O      -3.372309    -3.635243    -0.821361     191.98
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 H      -2.799137    -4.247812    -1.594798      24.74
 H      -3.062942    -2.061014     0.783081      23.22
 H      -1.633851    -2.729895    -0.177648      25.04
 C       1.396398     0.065522    -1.293112      52.68
 H       2.000022    -0.020413    -2.266435      21.37
 C       1.317665     1.197458     0.852127      72.87
 H       1.969621     1.779813     1.527453      19.33
 C      -0.087503     1.022361     0.887238      10.75
 O      -0.878631     1.292900     1.894986     232.31
 C      -0.609518     2.384747     2.830099     117.44
 H      -0.640780     3.330247     2.389739      25.81
 H      -1.454559     2.562698     3.592056      22.13
 H       0.438704     2.202924     3.421454      22.82
 C      -0.723450     0.184116    -0.181509       8.72
 O      -2.053424    -0.212846     0.037768     187.74
 C       0.080914    -0.138512    -1.317426      62.41
 H      -0.585489    -0.448463    -2.197219      19.79
 C       2.136672     0.636267    -0.267965      30.12
 C       3.693083     0.794916    -0.172941      83.65
 H       4.167117     0.244226    -1.099827      19.18
 O       4.087788     2.157308    -0.637355     214.00
 H       5.080980     2.080258    -0.813262      24.19
 C       4.462141     0.341004     1.111669     114.40
 H       4.463034     0.950341     1.973990      20.31
 O       3.917782    -0.755640     1.767786     299.36
 H       4.656257    -1.537801     1.862183      23.77
 C       5.934855     0.194381     1.061868      90.55
 O       6.517951     1.769795     0.678218     230.05
 H       6.839272     2.320196     1.403295      33.81
 H       6.439850    -0.528105     0.245341      27.51
 H       6.194742    -0.114862     1.972755      30.45
55
name= lig-ACN-Water-frame_916
 C      -3.821878     0.575981    -3.501209      90.50
 H      -3.729329    -0.347090    -4.036042      27.14
 C      -4.031877     1.935215    -1.514532      42.79
 H      -3.968467     2.140470    -0.367417      21.85
 C      -4.111851     3.251247    -2.115528     -37.63
 O      -4.090882     4.511964    -1.736167     224.87
 C      -3.054040     4.854070    -0.552473      59.27
 H      -2.259709     4.148996    -0.755240      28.27
 H      -3.882067     4.689293     0.303878      19.67
 H      -2.594861     5.780850    -1.296473      20.77
 C      -4.033509     3.150725    -3.660553     -37.78
 O      -3.881816     4.324582    -4.416281     179.84
 H      -3.417866     4.991453    -3.890569      24.44
 C      -3.825339     1.861934    -4.245920      35.30
 H      -3.610252     1.886794    -5.359585      18.96
 C      -3.916119     0.615347    -2.172044      45.94
 C      -4.047056    -0.555695    -1.173987     104.82
 H      -4.559780    -1.417424    -1.823491      26.18
 O      -4.907197    -0.462083    -0.094537     181.41
 H      -4.652724     0.261355     0.624549      24.23
 C      -2.753023    -1.176275    -0.927190      75.99
 H      -2.023605    -1.254958    -1.665949      27.48
 C      -2.650948    -2.566596    -0.061952      93.76
 O      -3.462400    -3.654807    -0.840742     175.29
 H      -2.849715    -3.586075    -1.669749      29.90
 H      -3.004735    -2.963454     1.019044      24.49
 H      -1.626509    -2.851043    -0.119840      27.68
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 C       1.512086     0.093080    -1.298719      27.92
 H       2.082238    -0.211702    -2.321895      19.71
 C       1.258268     1.256445     0.712304      68.77
 H       1.511475     1.979352     1.427686      21.03
 C      -0.056677     0.895421     0.813730      21.02
 O      -0.987329     1.298481     1.897592     207.02
 C      -0.602722     2.461226     2.727363      97.24
 H      -0.430084     3.250350     2.037491      27.83
 H      -1.304155     2.452118     3.571345      24.63
 H       0.521662     2.199303     3.126433      23.16
 C      -0.683802     0.190392    -0.138878      24.18
 O      -2.045421    -0.138107     0.053772     102.04
 C       0.048584    -0.081451    -1.299402      49.89
 H      -0.370357    -0.266665    -2.425324      23.92
 C       2.190585     0.676431    -0.180694      22.46
 C       3.676172     0.848475    -0.358653      80.09
 H       3.851278    -0.063604    -1.043707      20.36
 O       4.093646     2.129134    -0.710763     240.93
 H       5.074368     2.193720    -0.646124      24.01
 C       4.581443     0.407647     1.208014      66.90
 H       4.347920     1.328009     1.635160      22.85
 O       3.851405    -0.825594     1.812003     283.43
 H       4.511622    -1.606553     1.952955      27.09
 C       6.187000     0.211401     1.062908     100.16
 O       6.580994     1.697139     0.668465     259.01
 H       6.839088     1.878901     1.654619      29.15
 H       6.506053    -0.304791     0.088100      27.77
 H       6.697357    -0.174098     1.858011      28.52
55
name= lig-ACN-Water-frame_917
 C      -3.866666     0.644773    -3.530283      19.43
 H      -3.784922    -0.276123    -4.083582      21.87
 C      -4.084091     2.029555    -1.507013      28.38
 H      -4.330871     1.951392    -0.353398      20.39
 C      -4.113227     3.164276    -2.328621      40.86
 O      -4.156893     4.510259    -1.748718     177.40
 C      -3.037214     4.802751    -0.617521      67.08
 H      -2.375316     3.992977    -0.368269      29.94
 H      -3.408725     5.122411     0.497897      23.35
 H      -2.577040     6.004993    -0.650592      22.93
 C      -3.847857     3.117033    -3.609991      -5.23
 O      -3.982350     4.285731    -4.416412     151.65
 H      -3.363576     5.008553    -3.992309      22.28
 C      -3.786355     1.857381    -4.201013      33.46
 H      -3.776129     1.891026    -5.339264      25.64
 C      -4.041800     0.745326    -2.039798     -36.72
 C      -4.123830    -0.683407    -1.351733      59.91
 H      -4.587414    -1.450332    -2.066438      22.96
 O      -4.947020    -0.493710    -0.081871     168.87
 H      -4.416964     0.193398     0.314427      30.55
 C      -2.620454    -1.254458    -0.700754      85.60
 H      -2.167931    -1.446122    -1.629906      28.82
 C      -2.654732    -2.743296     0.010267     109.66
 O      -3.453307    -3.558764    -0.850472     220.82
 H      -3.113730    -3.609354    -1.646250      35.37
 H      -3.215517    -2.359572     1.092299      24.51
 H      -1.684804    -3.073378     0.125419      28.81
 C       1.537346     0.098550    -1.322753      51.62
 H       2.190624    -0.410437    -2.210651      22.98
 C       1.273153     1.413611     0.824138      32.81
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 H       1.747736     1.973925     1.608412      21.86
 C      -0.144459     0.885055     0.924312     -16.43
 O      -1.030925     1.291224     1.858924     177.55
 C      -0.497898     2.484825     2.595923     112.34
 H      -0.676398     3.438055     2.100154      27.47
 H      -1.307577     2.675260     3.262211      27.79
 H       0.439757     2.429423     3.338546      24.32
 C      -0.715417     0.103104    -0.254884       9.60
 O      -2.063351    -0.120232     0.020867     166.42
 C       0.143954    -0.044824    -1.359831      73.80
 H      -0.376016    -0.688479    -2.288790      25.36
 C       2.180527     0.725572    -0.295797       0.06
 C       3.795708     0.686484    -0.304877      64.91
 H       4.309127     0.192216    -1.183074      22.48
 O       4.084709     2.168214    -0.796472     240.80
 H       4.947811     2.349018    -0.373700      26.42
 C       4.572704     0.370024     1.169796      79.22
 H       4.411006     1.152751     1.888175      25.61
 O       3.856888    -0.808306     1.812408     332.93
 H       4.492815    -1.438893     1.748263      32.14
 C       6.229412     0.319887     0.894997     110.08
 O       6.694312     1.561182     0.751589     281.59
 H       7.071817     1.984951     1.556631      29.78
 H       6.307595    -0.373155     0.022467      28.77
 H       6.804315    -0.213655     1.646936      27.73
55
name= lig-ACN-Water-frame_918
 C      -3.912965     0.731936    -3.420133      76.01
 H      -4.017976    -0.255163    -3.895746      27.33
 C      -4.209792     2.011498    -1.406255      -0.85
 H      -4.465154     2.450121    -0.353596      18.78
 C      -3.996342     3.237464    -2.195990     -67.75
 O      -4.114365     4.491265    -1.637820     240.57
 C      -3.149399     4.783267    -0.661407      77.73
 H      -2.470526     3.934381    -0.680371      28.70
 H      -3.854297     4.904832     0.233910      21.84
 H      -2.325707     5.623927    -1.289879      21.85
 C      -3.747384     3.118138    -3.717509     -30.11
 O      -4.033058     4.209164    -4.434345     165.92
 H      -3.824937     5.096953    -4.091394      19.75
 C      -3.733283     1.853614    -4.367243      84.02
 H      -3.629406     1.600924    -5.466882      27.51
 C      -4.090300     0.694260    -2.096286      15.33
 C      -4.119744    -0.700784    -1.281774      66.94
 H      -4.727672    -1.390834    -1.884370      26.46
 O      -4.985794    -0.537652    -0.136455     194.98
 H      -4.536054    -0.235719     0.678504      28.43
 C      -2.580389    -1.338634    -0.711387      92.04
 H      -1.901873    -1.461635    -1.531538      27.24
 C      -2.711218    -2.643616     0.045931     108.81
 O      -3.471381    -3.490202    -0.832946     237.17
 H      -2.752728    -3.698450    -1.423066      31.86
 H      -3.527543    -2.701914     1.071649      23.99
 H      -1.893858    -3.133984     0.416581      29.61
 C       1.528059     0.110901    -1.354268      -8.68
 H       2.206971    -0.332376    -2.228470      21.85
 C       1.340423     1.250680     0.782369      74.24
 H       1.813840     1.780446     1.635509      21.93
 C      -0.028062     0.967801     0.809994      20.71
 O      -0.973698     1.358937     1.859111     215.16
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 C      -0.605114     2.568089     2.577744     112.59
 H      -0.137953     3.151569     1.746132      26.31
 H      -1.237235     2.753139     3.394401      26.44
 H       0.451491     2.206270     2.916769      24.78
 C      -0.577126     0.217440    -0.193583      -8.60
 O      -2.082932    -0.192842    -0.051262     144.35
 C       0.125050    -0.163551    -1.412837      46.68
 H      -0.285322    -0.958006    -2.254727      21.99
 C       2.150362     0.818903    -0.214337       2.00
 C       3.820697     0.758926    -0.173267      94.71
 H       4.061234    -0.095043    -0.843933      24.34
 O       4.097570     2.140842    -0.780069     203.04
 H       4.884377     2.675420    -0.453424      25.73
 C       4.531092     0.343570     1.069896     104.92
 H       4.497977     1.201072     1.788611      25.34
 O       3.969292    -0.761906     1.746435     301.08
 H       4.301211    -1.694287     1.524735      27.79
 C       6.026842     0.163055     0.785457      78.04
 O       6.869182     1.610837     0.779130     159.60
 H       7.200043     1.506680     1.684726      27.22
 H       6.288047    -0.062121    -0.208605      28.16
 H       6.345374    -0.558431     1.598195      27.22
55
name= lig-ACN-Water-frame_919
 C      -3.916293     0.674359    -3.490663      30.62
 H      -3.915550    -0.336662    -3.995773      25.04
 C      -4.271192     2.026929    -1.424521      73.21
 H      -4.491566     1.846806    -0.363556      22.66
 C      -3.882867     3.120706    -2.188058      -0.25
 O      -4.168294     4.415299    -1.674726     224.75
 C      -3.135974     4.753856    -0.676257      78.11
 H      -2.546801     3.928944    -0.267724      28.49
 H      -3.424656     5.283870     0.279626      23.76
 H      -2.450442     5.878351    -1.052611      22.00
 C      -3.791554     3.064326    -3.639904     -13.73
 O      -4.053173     4.237368    -4.545518     146.56
 H      -4.219118     4.873592    -3.854035      26.64
 C      -3.694235     1.839483    -4.316636      53.72
 H      -3.576340     1.878694    -5.421744      21.33
 C      -4.085915     0.733581    -1.952969     -10.08
 C      -4.075827    -0.633454    -1.192232      99.22
 H      -4.299866    -1.416722    -1.876257      26.64
 O      -5.052570    -0.617566    -0.125018     191.85
 H      -4.518165    -0.383698     0.740489      25.35
 C      -2.656238    -1.248672    -0.890905      70.76
 H      -2.143939    -1.714272    -1.757488      24.63
 C      -2.854874    -2.512304     0.135193      93.62
 O      -3.470711    -3.513979    -0.822853     106.20
 H      -2.848380    -3.811201    -1.703502      24.29
 H      -3.585109    -2.225275     1.205429      22.41
 H      -1.887780    -2.738849     0.397526      27.22
 C       1.555406     0.156431    -1.341599      53.90
 H       2.181082    -0.039350    -2.261018      24.31
 C       1.426951     1.111692     0.853098      35.90
 H       1.857496     1.612686     1.791453      20.21
 C      -0.063516     1.091162     0.741671     -10.82
 O      -0.903533     1.390620     1.796724     195.16
 C      -0.486648     2.609328     2.528147     123.27
 H      -0.542384     3.641831     2.018644      24.62
 H      -1.438611     2.913271     2.990408      25.14
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 H       0.202640     2.493659     3.419858      24.71
 C      -0.694698     0.183845    -0.280212       9.25
 O      -1.894841    -0.176657    -0.034666     123.56
 C       0.196213    -0.265397    -1.272059      73.12
 H      -0.292287    -0.781286    -2.194405      26.15
 C       2.203690     0.705575    -0.266232      55.60
 C       3.586432     0.895744    -0.228042      99.49
 H       3.944378     0.243533    -1.064030      25.20
 O       4.136202     2.104215    -0.713505     212.01
 H       5.032430     2.044933    -0.311676      29.41
 C       4.531083     0.496451     1.059991      87.39
 H       4.519907     1.306137     1.887685      22.93
 O       4.037216    -0.792724     1.694510     235.84
 H       4.428697    -1.456416     0.920735      26.46
 C       5.976613     0.167379     0.635862      96.61
 O       6.919234     1.478446     0.877010     146.25
 H       7.484955     1.436461     1.725664      24.96
 H       5.982787    -0.284035    -0.270890      30.67
 H       6.550555    -0.571383     1.341716      26.61
55
name= lig-ACN-Water-frame_920
 C      -3.842120     0.579829    -3.451419      80.43
 H      -3.745350    -0.432429    -3.962303      25.32
 C      -4.192413     1.901198    -1.406156      40.62
 H      -4.429765     2.280390    -0.475614      22.36
 C      -3.985745     3.130700    -2.272739     -25.32
 O      -4.179272     4.340971    -1.692328     190.42
 C      -3.089235     4.867093    -0.582162      51.94
 H      -2.541309     3.943876    -0.289363      26.53
 H      -3.797286     5.295025     0.055528      23.32
 H      -2.134345     5.481884    -1.378635      21.39
 C      -3.902790     3.107376    -3.651568      30.43
 O      -4.019468     4.162231    -4.464278     183.34
 H      -4.421698     5.016191    -4.089210      29.27
 C      -3.711072     1.783402    -4.136693      46.12
 H      -3.665575     1.693055    -5.217798      18.54
 C      -4.037279     0.675601    -2.113044      35.54
 C      -4.095273    -0.550313    -1.285099      91.56
 H      -4.616530    -1.212776    -1.881179      27.52
 O      -5.069209    -0.718609    -0.069958     137.70
 H      -4.869183    -0.057827     0.668283      27.08
 C      -2.758660    -1.072916    -0.797891      99.29
 H      -2.227817    -1.107892    -1.821774      26.83
 C      -2.909382    -2.358435    -0.056051     102.16
 O      -3.471450    -3.542566    -0.671499     179.45
 H      -2.777551    -3.405363    -1.572180      24.72
 H      -3.819054    -2.079451     0.831023      21.62
 H      -2.063877    -2.647235     0.497424      27.55
 C       1.541147     0.104513    -1.395334      44.41
 H       2.046763    -0.018627    -2.298773      24.28
 C       1.303391     1.065797     0.895903      75.80
 H       1.887247     1.370745     1.823891      21.54
 C      -0.010793     1.020477     0.719852      32.78
 O      -0.800416     1.505594     1.731188     195.13
 C      -0.567000     2.724283     2.572262      95.14
 H       0.055101     3.441879     1.795789      23.80
 H      -1.539842     2.755510     3.107949      24.24
 H       0.176377     2.479803     3.326637      26.41
 C      -0.566155     0.256157    -0.279450       5.21
 O      -1.911204    -0.235287    -0.024350     130.13
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 C       0.289215    -0.324987    -1.281887      71.90
 H      -0.149601    -0.890897    -2.089592      28.02
 C       2.112096     0.681981    -0.185473      -4.68
 C       3.710562     0.802443    -0.328119      84.17
 H       4.043171     0.024791    -1.018668      24.61
 O       4.205298     2.227897    -0.612437     221.71
 H       5.165674     2.210577    -0.560014      28.92
 C       4.424651     0.517965     1.056367      79.30
 H       4.331461     1.271546     1.996089      22.45
 O       4.098984    -0.767011     1.584279     304.58
 H       4.344018    -1.508753     1.020957      29.23
 C       6.080657     0.299813     0.614964      68.98
 O       6.892085     1.262581     0.873690     191.03
 H       7.087457     1.231283     1.914972      26.20
 H       6.201039     0.216465    -0.380814      30.01
 H       6.192334    -0.754490     1.195076      26.13
55
name= lig-ACN-Water-frame_921
 C      -3.713938     0.544692    -3.431023      28.69
 H      -3.676737    -0.441277    -4.001003      23.32
 C      -4.033543     1.957253    -1.538905      67.73
 H      -4.158271     1.820913    -0.548234      26.40
 C      -4.171465     3.135596    -2.180403      41.84
 O      -4.119400     4.410048    -1.593790     238.40
 C      -3.176548     4.827749    -0.684460     103.58
 H      -2.772003     4.094929     0.067358      28.20
 H      -3.509964     5.583697    -0.085124      25.92
 H      -2.226370     5.740585    -1.260373      22.52
 C      -3.989966     2.976731    -3.610680      -7.29
 O      -3.991801     4.132342    -4.449316     132.00
 H      -4.144757     4.844152    -3.734413      20.88
 C      -3.751048     1.733778    -4.233994      78.05
 H      -3.558578     1.659681    -5.292307      28.77
 C      -4.072411     0.657621    -2.031577      22.60
 C      -4.299982    -0.625673    -1.222508     109.77
 H      -4.381383    -1.418968    -1.868754      29.02
 O      -5.082967    -0.705080    -0.101437     246.17
 H      -4.969734     0.056019     0.453922      28.29
 C      -2.711880    -0.986727    -0.919115      64.67
 H      -2.105950    -1.287148    -1.857623      26.47
 C      -2.945694    -2.299076    -0.059148      96.04
 O      -3.423101    -3.527508    -0.607789     194.42
 H      -3.113921    -3.997009    -1.447279      27.68
 H      -3.805249    -2.034707     0.838131      22.12
 H      -1.962516    -2.393341     0.416388      27.94
 C       1.665758     0.084436    -1.372419      35.49
 H       2.306258    -0.225189    -2.090148      25.83
 C       1.477008     1.054668     0.859537      33.16
 H       1.737684     1.456484     1.865573      23.14
 C      -0.043703     0.996042     0.834250     -12.20
 O      -0.877152     1.609764     1.721729     173.75
 C      -0.547625     2.714618     2.555817     115.15
 H      -0.201543     3.767255     1.961658      24.33
 H      -1.439319     3.337243     2.934055      25.18
 H       0.061705     2.403013     3.374834      26.89
 C      -0.608013     0.147059    -0.288443     -12.02
 O      -1.959823    -0.167018     0.083415     101.27
 C       0.149524    -0.370850    -1.395997      55.12
 H      -0.162732    -1.180724    -1.961614      25.00
 C       2.272558     0.717066    -0.278717      42.89
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 C       3.793139     0.790295    -0.254382      93.98
 H       4.128547     0.256026    -1.116255      27.48
 O       4.207329     2.307096    -0.554688     176.37
 H       5.192788     2.416393    -0.704234      26.31
 C       4.530655     0.389994     0.929487     108.11
 H       4.177958     1.339351     1.579992      23.46
 O       4.041607    -0.791029     1.543684     278.03
 H       4.546556    -1.471695     1.155972      31.74
 C       5.898823     0.239455     0.543820      81.84
 O       7.046022     1.255389     0.993242     162.86
 H       7.108620     1.540957     1.961099      25.31
 H       5.844104     0.127350    -0.444587      29.41
 H       6.413223    -0.803985     0.833013      26.57
55
name= lig-ACN-Water-frame_922
 C      -3.716723     0.548500    -3.462383      62.98
 H      -3.533545    -0.494670    -3.804586      24.37
 C      -4.022540     1.896342    -1.346039      18.97
 H      -3.860615     2.106594    -0.345877      21.65
 C      -4.144806     3.148046    -2.211527      -9.57
 O      -4.219968     4.465965    -1.614003     227.14
 C      -3.159939     4.921383    -0.643643      72.45
 H      -2.868573     4.028341    -0.011155      24.48
 H      -3.608077     5.683343    -0.218401      24.09
 H      -1.931916     4.947410    -1.465635      20.36
 C      -4.046240     2.955303    -3.619302      -3.56
 O      -3.994643     4.096711    -4.383719     222.71
 H      -3.699670     4.854144    -3.917973      26.13
 C      -3.766879     1.666381    -4.298005      65.19
 H      -3.459973     1.836423    -5.323533      26.53
 C      -4.124435     0.640560    -2.112451      24.43
 C      -4.160812    -0.680802    -1.276609      94.05
 H      -4.771752    -1.362707    -1.798255      23.03
 O      -5.193988    -0.627520    -0.142894     189.24
 H      -4.721383    -0.165823     0.650101      23.25
 C      -2.797518    -1.141248    -0.898617      59.85
 H      -2.238408    -1.136531    -1.927500      20.82
 C      -2.801875    -2.314440     0.033783      93.70
 O      -3.425279    -3.556011    -0.589812     229.16
 H      -2.809100    -3.506476    -1.220586      31.88
 H      -3.497203    -1.983513     0.979289      21.00
 H      -1.805102    -2.669480     0.444322      24.98
 C       1.635883    -0.020366    -1.352067      32.13
 H       2.106211    -0.485711    -2.137114      24.13
 C       1.494878     1.122267     0.839879      63.07
 H       2.147039     1.675509     1.465735      22.39
 C       0.097386     0.948084     0.773008     -18.06
 O      -1.020565     1.640430     1.680180      98.34
 C      -0.498582     2.799123     2.549295      86.39
 H       0.296482     3.484447     1.821862      22.73
 H      -1.579916     2.943694     2.900039      22.64
 H       0.022248     2.536099     3.419505      27.53
 C      -0.656233     0.076224    -0.170640       6.86
 O      -2.003427    -0.065858     0.062458      68.17
 C       0.186021    -0.282479    -1.298372      55.55
 H      -0.109991    -0.936826    -2.058814      22.90
 C       2.303621     0.706067    -0.329788      24.18
 C       3.791150     0.943245    -0.423805      93.90
 H       4.134100     0.422465    -1.299432      26.30
 O       4.152287     2.313149    -0.498956     238.42
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 H       5.120778     2.226484    -0.610961      30.21
 C       4.548603     0.370428     0.972445      64.64
 H       4.817319     1.028147     1.931539      23.00
 O       3.926718    -0.879905     1.541645     231.42
 H       4.583760    -1.746728     1.607921      25.07
 C       6.117039     0.193681     0.474285      68.42
 O       7.117526     1.241312     1.019688     132.58
 H       7.152102     1.140701     1.987244      28.54
 H       6.385227     0.356653    -0.516446      28.40
 H       6.430949    -0.861393     0.901334      27.75
55
name= lig-ACN-Water-frame_923
 C      -3.861363     0.541732    -3.478484      34.64
 H      -3.632388    -0.378708    -4.007952      21.74
 C      -4.113452     1.946979    -1.350336      65.97
 H      -4.196782     1.859120    -0.253231      19.82
 C      -4.030715     3.031015    -2.114464       2.41
 O      -4.336595     4.420362    -1.724261     146.53
 C      -3.129824     4.876168    -0.665190      73.89
 H      -3.186540     4.269402     0.230346      27.59
 H      -3.210876     5.845892    -0.407208      26.36
 H      -1.814578     5.161717    -1.306201      21.30
 C      -3.995639     2.963689    -3.595547      13.99
 O      -4.011571     4.085500    -4.402838     185.15
 H      -3.691877     4.865696    -3.849099      25.22
 C      -3.773630     1.776876    -4.235128      49.05
 H      -3.528387     1.550383    -5.283392      19.58
 C      -4.024400     0.659287    -2.047348      26.15
 C      -4.179927    -0.632721    -1.316260      86.97
 H      -4.331937    -1.439798    -2.065029      25.97
 O      -5.206237    -0.551862    -0.195101     161.48
 H      -4.759726    -0.259122     0.747560      21.05
 C      -2.775019    -1.237222    -0.752511      74.25
 H      -2.036908    -1.551240    -1.610042      22.76
 C      -2.686349    -2.489686     0.165032      95.00
 O      -3.348500    -3.505807    -0.570738     257.85
 H      -3.152248    -3.837035    -1.379524      31.67
 H      -3.264271    -2.349539     1.176022      23.60
 H      -1.504104    -2.649317     0.346311      24.47
 C       1.565920    -0.123966    -1.311155      57.39
 H       2.058515    -0.321288    -2.265853      25.24
 C       1.466577     1.242870     0.691909      67.03
 H       1.709842     1.905080     1.403626      23.49
 C       0.019160     0.988463     0.854787       8.29
 O      -0.902038     1.608465     1.584316     189.42
 C      -0.531695     2.736331     2.502167     109.87
 H       0.100064     3.608137     1.776308      23.55
 H      -1.164658     3.655071     2.837618      24.01
 H       0.067089     2.305889     3.236645      28.01
 C      -0.526450     0.143331    -0.078514       9.09
 O      -2.066312    -0.032577    -0.097160      83.37
 C       0.171002    -0.281009    -1.142859      54.57
 H      -0.432703    -0.523246    -2.016735      22.45
 C       2.189613     0.665495    -0.333313      29.38
 C       3.769357     0.918384    -0.373647      85.29
 H       4.218254     0.380115    -1.227840      25.29
 O       4.135521     2.372680    -0.484459     251.30
 H       5.069248     2.572130    -0.443502      28.81
 C       4.660267     0.270270     0.946992      46.35
 H       4.383686     1.171791     1.665346      24.25
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 O       3.856585    -0.889252     1.475951     246.79
 H       4.578086    -1.652474     1.720333      26.21
 C       6.410205     0.152564     0.466999      92.06
 O       7.114944     1.171523     1.036764     212.35
 H       7.428363     1.117153     1.973964      24.41
 H       6.408355     0.032126    -0.629549      28.45
 H       6.767632    -0.914994     0.739486      28.57
55
name= lig-ACN-Water-frame_924
 C      -3.968200     0.626532    -3.409387      59.90
 H      -4.225530    -0.304901    -3.845051      25.99
 C      -4.179809     1.834157    -1.405451      28.97
 H      -4.716582     1.945063    -0.372957      21.52
 C      -4.050263     3.136614    -2.193449      14.73
 O      -4.224190     4.366755    -1.674353     248.41
 C      -3.249887     4.882474    -0.801313      87.17
 H      -3.265706     4.361470     0.145492      26.98
 H      -3.475442     5.919444    -0.745074      25.38
 H      -2.136473     4.154108    -1.347986      23.94
 C      -3.826796     3.019709    -3.535155      -0.81
 O      -4.023927     4.116493    -4.413586     168.43
 H      -4.263230     4.971026    -3.858311      23.28
 C      -3.769616     1.729542    -4.175719      53.12
 H      -3.894641     1.961523    -5.261196      24.41
 C      -3.921175     0.635480    -2.011698      32.91
 C      -4.129550    -0.702894    -1.201315      81.39
 H      -4.685011    -1.419362    -1.912677      24.65
 O      -5.151639    -0.547891    -0.310400     193.64
 H      -4.635962    -0.113794     0.521398      23.31
 C      -2.619589    -1.184567    -0.612082      83.58
 H      -2.317795    -1.556685    -1.653270      24.96
 C      -2.597493    -2.581827     0.230925      93.18
 O      -3.342910    -3.589171    -0.517954     202.57
 H      -2.745045    -3.394599    -1.359944      26.28
 H      -2.961121    -2.692633     1.288951      25.26
 H      -1.414039    -2.933033     0.240785      24.45
 C       1.554874    -0.133921    -1.265544      32.88
 H       2.111459    -0.445791    -2.247055      23.80
 C       1.319830     1.400218     0.673856      56.48
 H       1.941795     1.969371     1.236383      24.51
 C       0.026734     1.041325     0.829505      15.55
 O      -0.903320     1.701596     1.656882     203.57
 C      -0.437117     2.723546     2.391888     107.78
 H       0.448428     3.404908     1.765879      24.58
 H      -1.566106     2.866665     2.687233      21.75
 H       0.027379     2.489641     3.368773      27.52
 C      -0.694497     0.129600    -0.081161      -2.61
 O      -1.997612     0.007277    -0.204516     156.80
 C       0.123805    -0.390105    -1.184471      34.90
 H      -0.534709    -0.836079    -2.050773      24.82
 C       2.263377     0.674071    -0.289869      -1.14
 C       3.797366     0.752651    -0.263573      88.12
 H       4.041587     0.481974    -1.337300      24.24
 O       4.088759     2.407435    -0.491850     142.65
 H       5.032210     2.443793    -0.137784      28.45
 C       4.681599     0.222286     0.810096      81.55
 H       4.961733     0.994254     1.676773      24.85
 O       3.904998    -0.840333     1.367031     299.72
 H       4.420696    -1.602154     1.461505      31.06
 C       6.361434    -0.042205     0.532431      74.88
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 O       7.195727     1.190920     1.042339      84.12
 H       7.171853     1.200606     2.096698      24.41
 H       6.433021     0.252558    -0.594264      25.54
 H       6.828469    -0.950282     0.900175      29.26
55
name= lig-ACN-Water-frame_925
 C      -3.962109     0.538841    -3.391214      32.55
 H      -4.236273    -0.329399    -3.952690      24.73
 C      -4.209680     1.945006    -1.449710      57.20
 H      -4.447795     2.122145    -0.306982      21.07
 C      -4.059260     3.040521    -2.173633       3.73
 O      -4.297544     4.336460    -1.669684     244.54
 C      -3.240174     4.817499    -0.831608     120.19
 H      -3.468931     4.766624     0.182318      28.32
 H      -3.091451     5.889042    -1.063267      26.39
 H      -1.895535     4.763910    -1.088603      23.59
 C      -3.720607     3.086557    -3.604647      31.29
 O      -4.018384     4.153899    -4.392179     188.17
 H      -4.498515     4.813292    -3.901417      25.31
 C      -3.818940     1.837298    -4.193577      17.93
 H      -4.063816     1.526075    -5.239591      25.70
 C      -3.945069     0.550530    -1.979903      15.24
 C      -3.982507    -0.762271    -1.191227      91.59
 H      -4.076227    -1.713919    -1.912685      23.69
 O      -5.144344    -0.546636    -0.266392     201.85
 H      -4.888617    -0.187018     0.630885      25.02
 C      -2.667216    -1.243216    -0.664800      86.87
 H      -1.974360    -1.435824    -1.491785      24.55
 C      -2.497687    -2.578964     0.270530      75.67
 O      -3.289172    -3.649225    -0.482643     153.97
 H      -3.082864    -3.953953    -1.546572      23.55
 H      -2.938713    -2.372941     1.221836      26.03
 H      -1.358818    -3.080497     0.402273      23.90
 C       1.523046    -0.112565    -1.186147      50.68
 H       2.212895    -0.826531    -1.858536      21.96
 C       1.432165     1.398283     0.635405      67.27
 H       1.619160     2.105883     1.434260      20.14
 C      -0.080401     1.056633     0.680182      -9.76
 O      -0.936988     1.626549     1.640363     141.13
 C      -0.409587     2.853418     2.510302      74.89
 H       0.069874     3.770658     1.732923      23.23
 H      -1.097498     3.735748     2.893210      23.33
 H       0.323814     2.423738     3.259894      24.69
 C      -0.560333     0.113564    -0.256277      28.35
 O      -2.032545     0.065040    -0.151624     117.84
 C       0.201012    -0.440203    -1.204565      70.51
 H       0.031314    -1.389169    -1.907999      23.42
 C       2.160545     0.656762    -0.205265      36.37
 C       3.789353     0.880120    -0.398422      81.23
 H       4.155241     0.109514    -1.188206      25.88
 O       4.059264     2.273801    -0.468695     219.83
 H       4.802364     2.570079     0.095702      27.27
 C       4.798060     0.218083     0.822228      70.46
 H       4.692925     1.060789     1.697173      24.11
 O       3.987640    -0.871343     1.288297     285.83
 H       4.429441    -1.707319     1.174332      29.37
 C       6.225424    -0.044810     0.549425      95.12
 O       7.181502     1.108135     1.033940     124.52
 H       7.131661     1.360156     2.046933      25.81
 H       6.740241    -0.418586    -0.455215      26.17
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 H       6.340888    -0.991015     1.048886      29.91
55
name= lig-ACN-Water-frame_926
 C      -3.868435     0.583679    -3.462899      67.92
 H      -3.611313    -0.374036    -3.918432      23.07
 C      -4.122219     1.811805    -1.399536      35.30
 H      -4.093203     1.927387    -0.272004      20.12
 C      -4.007701     3.070510    -2.260627     -20.45
 O      -4.417637     4.277070    -1.703944     154.91
 C      -3.084558     5.001123    -0.755264      43.41
 H      -3.407504     4.841953     0.237028      24.73
 H      -3.249221     6.063820    -1.144752      22.11
 H      -2.412047     3.928523    -1.004095      23.15
 C      -3.848871     2.975934    -3.637193      -4.62
 O      -4.002878     4.247461    -4.397296     150.91
 H      -4.170762     4.851658    -3.654750      23.39
 C      -3.889872     1.665180    -4.200302      50.20
 H      -3.786651     1.825027    -5.295762      27.69
 C      -4.025266     0.611968    -2.020040      27.98
 C      -4.013152    -0.783126    -1.216000      78.04
 H      -4.566884    -1.485192    -2.021278      23.10
 O      -5.118287    -0.631330    -0.214773     192.22
 H      -4.606453    -0.406330     0.558222      27.56
 C      -2.515208    -1.229868    -0.709141      90.76
 H      -2.144393    -1.532816    -1.690190      23.69
 C      -2.566620    -2.544082     0.127138     105.96
 O      -3.235644    -3.687612    -0.380476     227.32
 H      -2.708524    -3.824626    -1.268155      26.74
 H      -3.048707    -2.494751     1.022175      26.34
 H      -1.339417    -2.633619     0.378496      23.62
 C       1.714526    -0.237595    -1.129339      32.92
 H       2.524211    -0.811904    -1.827766      22.83
 C       1.277569     1.341595     0.719709      64.73
 H       1.877032     2.034205     1.403856      19.45
 C      -0.022674     1.197980     0.614479      17.62
 O      -0.947527     1.617675     1.636335     141.26
 C      -0.375196     2.988262     2.507109      51.41
 H       0.189167     3.437039     1.539617      22.11
 H      -1.305701     3.168775     3.154618      22.76
 H       0.486134     2.491200     3.214442      23.18
 C      -0.648314     0.229028    -0.311535      -7.86
 O      -1.992559    -0.010689    -0.060309     136.86
 C       0.295557    -0.560882    -1.222726      45.22
 H      -0.172783    -1.500870    -1.774909      20.39
 C       2.284125     0.704946    -0.246895      18.44
 C       3.759939     0.834450    -0.389825     103.54
 H       3.980736     0.648901    -1.523436      24.72
 O       4.061331     2.245544    -0.500327     197.74
 H       4.569320     2.389028     0.307276      32.68
 C       4.617061     0.339441     0.780249      76.12
 H       4.547237     1.104111     1.722921      24.86
 O       4.073458    -0.961719     1.229819     227.73
 H       4.799894    -1.767747     1.088187      25.39
 C       6.237078    -0.047767     0.686825      96.10
 O       7.106755     0.948945     0.975336     219.50
 H       7.110584     1.044860     1.932159      29.16
 H       6.160765    -0.396445    -0.437723      26.41
 H       6.428729    -0.717312     1.426676      30.59
55
name= lig-ACN-Water-frame_927
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 C      -3.752182     0.461468    -3.447743      43.06
 H      -3.553988    -0.550675    -3.910985      24.56
 C      -3.957546     1.861682    -1.443008      58.90
 H      -4.155459     1.902333    -0.402951      23.44
 C      -4.084467     2.990724    -2.165178      -4.28
 O      -4.369481     4.301994    -1.646924     197.54
 C      -3.192126     4.994835    -0.779505      74.22
 H      -3.510369     5.139893     0.268577      24.35
 H      -2.662405     5.975258    -1.244063      22.34
 H      -2.000043     4.413347    -1.058514      21.32
 C      -4.092500     2.979735    -3.673795       0.87
 O      -3.980511     4.177099    -4.326302     150.70
 H      -3.892307     4.920094    -3.609947      22.66
 C      -3.845876     1.727532    -4.389424      35.87
 H      -3.572286     1.453202    -5.404565      26.31
 C      -4.010968     0.546372    -2.103974      34.11
 C      -4.163790    -0.681018    -1.297990      86.89
 H      -4.444225    -1.648499    -1.968046      21.93
 O      -5.005836    -0.775009    -0.156109     273.86
 H      -4.635263    -0.342138     0.581757      26.88
 C      -2.647686    -1.169977    -0.887846      71.42
 H      -1.958757    -1.188319    -1.693555      22.75
 C      -2.605719    -2.418633     0.128600      91.30
 O      -3.135538    -3.725627    -0.371192     250.58
 H      -2.872366    -3.978101    -1.177601      30.91
 H      -3.001300    -2.067691     0.957272      25.97
 H      -1.478638    -2.864901     0.341474      22.47
 C       1.765538    -0.397643    -1.098438      46.46
 H       2.379680    -0.852531    -1.989218      22.65
 C       1.450710     1.306414     0.670766      56.60
 H       1.766671     1.861097     1.606947      18.18
 C      -0.122900     1.215901     0.619641      -7.89
 O      -0.885975     1.739977     1.645554     189.64
 C      -0.375329     2.822174     2.377575     116.09
 H      -0.368831     3.972965     1.988709      23.61
 H      -1.305525     3.117345     2.931022      24.14
 H       0.526853     2.767287     3.206796      23.23
 C      -0.563330     0.263130    -0.363081      23.59
 O      -1.879672    -0.213957    -0.035204     166.20
 C       0.343788    -0.526702    -1.043212      58.33
 H      -0.054740    -1.248034    -1.808362      22.11
 C       2.204300     0.664396    -0.280101      34.88
 C       3.744243     0.843921    -0.393171      62.84
 H       4.146006     0.085283    -1.207209      23.91
 O       4.118995     2.387132    -0.497121     150.06
 H       4.347263     2.755681     0.417762      28.08
 C       4.507076     0.227906     0.845759      82.96
 H       4.243931     1.063904     1.698506      23.76
 O       4.069654    -1.017248     1.167985     243.53
 H       4.895945    -1.644477     1.269617      25.02
 C       6.010583    -0.100608     0.778964      92.11
 O       7.125991     0.916143     0.930295     195.19
 H       7.396593     1.258286     1.836250      27.77
 H       6.436639    -0.490747    -0.258885      27.47
 H       6.197284    -0.937103     1.301380      32.16
55
name= lig-ACN-Water-frame_928
 C      -3.717962     0.537373    -3.624414      61.33
 H      -3.887856    -0.458779    -4.146573      24.84
 C      -3.945384     1.823696    -1.470759      39.29
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 H      -3.908459     1.887913    -0.444556      25.03
 C      -4.192109     3.035023    -2.239919      -7.97
 O      -4.203067     4.320975    -1.570896     218.76
 C      -3.226952     4.949271    -0.912066      96.58
 H      -3.728490     5.201183     0.133184      23.00
 H      -3.326864     6.021226    -1.468303      20.24
 H      -2.338436     4.140962    -0.426645      23.56
 C      -4.133931     2.877889    -3.637521     -10.82
 O      -3.993247     4.100070    -4.287272     121.33
 H      -4.147709     4.807709    -3.575542      22.51
 C      -3.758210     1.663992    -4.289720      75.41
 H      -3.701331     1.866476    -5.335272      21.98
 C      -3.955946     0.602605    -2.141802      20.22
 C      -4.080997    -0.751502    -1.306718      81.83
 H      -4.534985    -1.509459    -2.132366      23.57
 O      -4.953244    -0.870937    -0.119504     212.06
 H      -4.554346    -0.458549     0.675583      25.18
 C      -2.695629    -1.188772    -1.008132      71.66
 H      -2.433335    -1.567232    -1.960711      23.51
 C      -2.585324    -2.386845     0.012307      97.76
 O      -3.113172    -3.731662    -0.341543     242.72
 H      -2.940880    -3.730877    -1.262843      30.39
 H      -3.157491    -2.299180     0.788393      26.07
 H      -1.463788    -2.170334     0.352585      23.19
 C       1.705304    -0.388236    -1.083806      57.46
 H       2.248800    -1.073882    -1.761764      23.60
 C       1.397803     1.313850     0.600196      79.69
 H       1.956171     1.929494     1.271327      22.82
 C       0.100983     1.177557     0.655277      32.13
 O      -0.825704     1.767419     1.514530     228.29
 C      -0.497786     2.879932     2.420587     100.14
 H      -0.233314     3.690823     1.551294      23.78
 H      -1.125239     2.870825     3.309313      25.46
 H       0.633628     2.482335     2.731398      24.53
 C      -0.534462     0.203144    -0.208251      16.14
 O      -1.830106    -0.316698    -0.028521      79.20
 C       0.287451    -0.572123    -1.022574      53.94
 H      -0.143586    -1.329733    -1.594208      25.07
 C       2.311839     0.573433    -0.303112      39.56
 C       3.793354     0.954640    -0.304828      77.93
 H       4.301608     0.723924    -1.330026      21.72
 O       4.154213     2.372616    -0.478282     242.50
 H       4.054195     2.765478     0.411061      32.36
 C       4.509759     0.236666     1.001802      79.01
 H       4.322434     0.741172     2.068042      24.06
 O       3.854551    -1.171411     1.112350     282.05
 H       4.397519    -1.783003     1.511195      30.97
 C       6.016527    -0.066789     0.768701     103.73
 O       7.113799     0.867823     0.925863     221.71
 H       6.893215     1.438692     1.797643      28.55
 H       5.900680    -0.599217    -0.274287      25.56
 H       6.190080    -0.628480     1.564398      29.83
55
name= lig-ACN-Water-frame_929
 C      -3.827644     0.471237    -3.561880      32.19
 H      -3.675032    -0.473154    -4.186049      23.77
 C      -4.040637     1.812605    -1.488314      82.91
 H      -3.762701     1.833652    -0.484612      26.41
 C      -4.132166     2.972604    -2.150943      40.46
 O      -4.266144     4.181784    -1.711013     231.03
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 C      -3.225154     5.006678    -0.828544      74.51
 H      -3.791729     5.415101     0.147866      22.58
 H      -2.480126     5.783616    -1.428666      23.47
 H      -2.124439     4.345739    -0.797780      24.90
 C      -3.990386     2.956085    -3.549368      16.63
 O      -4.057191     4.055013    -4.330759     189.59
 H      -4.448414     4.786023    -3.905141      29.01
 C      -3.756867     1.810891    -4.294020      44.83
 H      -3.615673     1.818397    -5.341896      22.27
 C      -3.897813     0.559739    -2.195280      35.63
 C      -4.003609    -0.742118    -1.324725     109.23
 H      -4.572420    -1.532135    -1.972489      26.53
 O      -4.933159    -0.903896    -0.163803     189.66
 H      -4.607925    -0.294512     0.679073      24.04
 C      -2.580913    -1.371064    -1.010626      77.89
 H      -1.843535    -1.326262    -1.750761      25.25
 C      -2.622420    -2.473962    -0.010559     108.65
 O      -3.056351    -3.703169    -0.391202     264.99
 H      -2.921717    -4.151799    -1.360945      25.12
 H      -3.026924    -1.979234     0.767156      26.66
 H      -1.530408    -2.817385     0.259845      23.75
 C       1.725140    -0.392698    -1.131033      40.48
 H       2.391292    -1.067217    -1.586531      23.00
 C       1.582810     1.401463     0.543473      58.75
 H       1.898120     2.273808     0.958011      24.98
 C       0.096692     1.060234     0.684255      -3.35
 O      -0.887272     1.754115     1.390880     142.12
 C      -0.413640     2.877054     2.379824      96.84
 H      -0.589463     4.110855     2.062910      23.08
 H      -1.255981     2.854682     3.053869      25.33
 H       0.628198     2.780262     2.986492      26.26
 C      -0.530996    -0.012351    -0.097737       3.96
 O      -1.919622    -0.251350    -0.058039      87.38
 C       0.232747    -0.674188    -1.086699      45.40
 H      -0.169950    -1.500763    -1.470896      26.64
 C       2.385628     0.604881    -0.282654      27.63
 C       3.883595     0.933864    -0.184303      90.43
 H       4.287038     0.272669    -1.029379      23.97
 O       4.148437     2.352008    -0.336011     232.86
 H       3.772428     2.910805     0.348884      31.04
 C       4.466101     0.211942     1.059267      77.23
 H       4.297570     0.844708     2.031753      25.82
 O       3.627361    -1.209708     1.036631     238.70
 H       4.251296    -1.732694     1.553695      29.31
 C       6.027268    -0.182823     0.866710     103.06
 O       7.032863     0.887520     0.893798     173.98
 H       6.941230     1.480600     1.735538      28.59
 H       6.327726    -0.636744    -0.159454      26.91
 H       6.254746    -0.966130     1.420302      32.03
55
name= lig-ACN-Water-frame_930
 C      -3.863583     0.571432    -3.568610      53.02
 H      -3.687092    -0.431966    -4.006791      22.91
 C      -4.046996     1.644834    -1.397252      48.21
 H      -4.275887     1.722249    -0.312543      23.61
 C      -3.967110     2.923736    -2.181467     -30.27
 O      -4.353721     4.325361    -1.688536     148.10
 C      -3.142650     4.939925    -0.861496      72.85
 H      -3.647626     5.528112     0.146089      22.72
 H      -2.973421     5.828173    -1.624489      21.65
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 H      -2.645033     3.983165    -0.228521      21.73
 C      -3.848223     2.981179    -3.609766      -2.17
 O      -4.142449     4.117739    -4.447114     133.65
 H      -4.384166     4.952858    -3.920471      20.57
 C      -3.780615     1.702776    -4.266128      49.05
 H      -3.611490     1.727405    -5.313341      26.25
 C      -3.943148     0.449750    -2.080746      42.61
 C      -3.933756    -0.870093    -1.390962     114.26
 H      -4.206478    -1.638163    -2.164226      27.91
 O      -4.883613    -0.851192    -0.256126     190.54
 H      -4.534226    -0.079513     0.459628      22.39
 C      -2.450288    -1.292079    -0.918650      79.93
 H      -1.960907    -1.534962    -1.893354      24.53
 C      -2.439582    -2.592063     0.065536      86.66
 O      -3.163638    -3.862581    -0.466109     211.51
 H      -2.694611    -3.724503    -1.453092      24.27
 H      -3.146414    -2.514310     0.865918      23.99
 H      -1.368014    -2.636312     0.482551      24.71
 C       1.777275    -0.391775    -1.097631      75.27
 H       2.275871    -0.900365    -1.845031      26.52
 C       1.417052     1.431414     0.515737      67.78
 H       1.669068     2.304914     1.053197      22.78
 C       0.120369     0.965226     0.613373     -17.50
 O      -0.846247     1.858655     1.365351     170.10
 C      -0.497466     2.819421     2.338090      91.93
 H      -0.482583     3.919089     1.660380      21.63
 H      -1.154602     2.677183     3.189567      24.60
 H       0.566642     2.496711     2.822470      24.92
 C      -0.484385    -0.168623    -0.096369     -19.10
 O      -2.011996    -0.157241    -0.068841      86.38
 C       0.435009    -0.782246    -1.051745      50.93
 H       0.316502    -1.519768    -1.768889      24.77
 C       2.302820     0.639257    -0.326955      24.13
 C       3.888858     0.772788    -0.175317      73.58
 H       4.549774     0.587520    -1.068261      25.24
 O       4.180199     2.325633    -0.184599     177.65
 H       3.626214     2.590382     0.612772      29.23
 C       4.453252     0.036117     1.064959      95.03
 H       4.197828     0.507917     2.039226      26.44
 O       3.557461    -1.085297     1.016894     262.21
 H       4.048478    -1.983204     1.415223      27.76
 C       6.005159    -0.355491     0.941627      92.51
 O       6.911917     0.944968     0.914125     138.57
 H       7.250427     1.086635     1.829414      27.52
 H       5.984401    -0.698605    -0.121892      29.61
 H       6.328915    -0.974770     1.668547      31.34
55
name= lig-ACN-Water-frame_931
 C      -3.798958     0.465985    -3.449865      42.07
 H      -3.976178    -0.349875    -4.106500      27.18
 C      -4.042540     1.750058    -1.410838      22.30
 H      -4.585416     1.739368    -0.368711      21.10
 C      -3.929518     3.008854    -2.211014     -42.34
 O      -4.315370     4.329992    -1.584442     219.53
 C      -3.283370     4.854112    -0.894793      95.47
 H      -3.763577     5.667665    -0.039248      22.75
 H      -2.258279     5.340836    -1.463071      22.90
 H      -2.351833     4.066041    -0.597016      21.94
 C      -3.848332     2.956076    -3.663491      -7.67
 O      -4.175113     4.120040    -4.505924     128.89
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 H      -4.099315     4.905764    -3.819183      22.10
 C      -3.766738     1.706593    -4.289670      27.98
 H      -3.886809     1.582415    -5.369662      26.57
 C      -3.968221     0.437453    -2.108778      27.27
 C      -3.873556    -1.027523    -1.363189     105.74
 H      -4.258301    -1.878688    -1.902787      23.11
 O      -4.831371    -0.812656    -0.373250     298.16
 H      -4.366330    -0.437278     0.436203      23.31
 C      -2.504477    -1.299556    -0.745436      91.13
 H      -1.743985    -1.422164    -1.582001      20.40
 C      -2.400080    -2.659030     0.128933      74.35
 O      -3.165475    -3.921214    -0.517876     213.57
 H      -3.059218    -4.235593    -1.487441      25.25
 H      -2.864015    -2.476950     1.190837      23.46
 H      -1.417407    -3.091240     0.246019      23.27
 C       1.878845    -0.402263    -1.094759      45.02
 H       2.642651    -0.711424    -1.803379      22.30
 C       1.293658     1.322668     0.437734      69.76
 H       1.727444     2.139448     1.092601      22.74
 C      -0.042902     1.013108     0.604375      27.60
 O      -0.854566     1.785780     1.244652     228.16
 C      -0.496664     2.741647     2.297311      99.46
 H      -0.271329     3.930230     1.923318      23.93
 H      -1.298915     2.881572     3.060560      25.58
 H       0.555975     2.445021     2.741035      25.79
 C      -0.471274    -0.107808    -0.153551       2.41
 O      -1.826262    -0.169519    -0.152676     184.95
 C       0.491502    -0.871527    -0.944602      69.96
 H      -0.094243    -1.579675    -1.591777      22.78
 C       2.335046     0.705717    -0.299860      17.91
 C       3.847269     0.908502    -0.250933      85.41
 H       4.082161     0.474898    -1.226218      24.27
 O       4.198052     2.213955    -0.002272     213.38
 H       3.968335     2.514242     0.897223      29.08
 C       4.464480    -0.058986     1.088885      75.33
 H       4.410623     0.615689     1.955112      25.97
 O       3.530570    -1.132680     1.052967     264.24
 H       4.000352    -2.013096     1.340412      27.06
 C       5.957213    -0.351387     0.948923     115.08
 O       6.758407     0.854296     0.960229     271.84
 H       6.889024     1.097575     1.963836      26.35
 H       6.302875    -1.055621     0.204968      29.15
 H       6.225710    -0.860722     1.830548      28.41
55
name= lig-ACN-Water-frame_932
 C      -3.745049     0.426205    -3.569215      35.42
 H      -3.678697    -0.550243    -3.911280      20.83
 C      -4.078622     1.845688    -1.572632      46.33
 H      -4.065950     2.100643    -0.393091      15.91
 C      -4.035759     3.026413    -2.230365      19.16
 O      -4.303513     4.154900    -1.611552     231.77
 C      -3.132663     4.828526    -0.849032      86.36
 H      -3.641970     5.737846    -0.027783      21.09
 H      -2.612809     5.437371    -1.751845      20.74
 H      -2.982644     4.007583     0.017583      19.29
 C      -3.942808     2.969991    -3.659445       9.95
 O      -4.136842     4.031571    -4.464716     189.09
 H      -4.225898     4.917359    -4.095733      27.80
 C      -3.782840     1.658010    -4.254002      50.86
 H      -3.947725     1.636869    -5.363504      23.49
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 C      -3.834271     0.477224    -2.104371      29.36
 C      -3.850484    -0.892878    -1.312015     105.50
 H      -4.025995    -1.616251    -2.060095      26.36
 O      -4.900003    -0.841626    -0.287958     261.62
 H      -4.525275    -0.565359     0.478545      31.77
 C      -2.420085    -1.486200    -0.753098      81.60
 H      -2.012848    -1.903900    -1.787213      20.86
 C      -2.462543    -2.810524     0.081051     110.97
 O      -3.166840    -3.869406    -0.419956     334.44
 H      -2.800094    -3.823771    -1.237507      33.72
 H      -2.646711    -2.601991     1.229154      23.96
 H      -1.397026    -2.977810     0.043979      24.30
 C       1.846341    -0.442109    -1.087076      49.98
 H       2.463965    -1.256101    -1.581093      19.49
 C       1.418163     1.354935     0.503176      62.95
 H       1.650143     2.360746     1.088358      18.41
 C       0.027406     1.060017     0.496897       1.16
 O      -1.067652     1.766947     1.219321     168.50
 C      -0.417552     2.704853     2.262102      97.88
 H      -0.304533     3.760575     1.675833      21.17
 H      -1.363256     2.660658     2.856706      22.97
 H       0.278861     2.238191     3.011563      25.15
 C      -0.380583    -0.058881    -0.271600      20.43
 O      -1.756447    -0.259074    -0.185518     173.75
 C       0.529165    -0.841979    -0.876994      57.97
 H       0.347006    -1.940246    -1.312381      21.48
 C       2.252986     0.627327    -0.329048      52.95
 C       3.753665     0.911979    -0.172309     101.32
 H       4.431349     0.743183    -0.976754      25.15
 O       4.269981     2.269385     0.140052     179.67
 H       4.355260     2.236226     1.098713      28.90
 C       4.376849     0.016774     0.896642      87.39
 H       4.172113     0.513626     1.832890      26.03
 O       3.550643    -1.305298     1.149252     282.44
 H       4.154124    -1.858720     1.496664      30.52
 C       5.932382    -0.425391     1.053132     112.72
 O       6.652560     0.770820     1.013566     304.23
 H       6.699987     1.449812     1.813924      25.98
 H       6.207618    -0.904360     0.161559      28.30
 H       5.976400    -1.073163     1.901811      29.35
55
name= lig-ACN-Water-frame_933
 C      -3.666601     0.459141    -3.552088      57.59
 H      -3.360248    -0.286873    -4.174042      23.72
 C      -3.999885     1.716652    -1.551517      43.09
 H      -3.931777     1.674124    -0.371681      17.24
 C      -4.140703     2.928012    -2.286381       1.69
 O      -4.316492     4.176576    -1.572471     234.85
 C      -3.139673     4.767785    -0.787216      70.58
 H      -3.775898     5.878667    -0.547554      21.47
 H      -2.134771     4.957957    -1.420621      23.83
 H      -2.410524     4.175239    -0.073121      22.51
 C      -4.032699     2.847939    -3.721242      -2.06
 O      -4.100950     3.996594    -4.514161     173.82
 H      -4.431270     4.645769    -3.901694      24.10
 C      -3.850852     1.618783    -4.300455      51.60
 H      -3.613891     1.702509    -5.408732      28.38
 C      -3.686915     0.555713    -2.139994      45.77
 C      -3.826572    -0.735075    -1.278157     113.58
 H      -4.422094    -1.276750    -1.894129      27.87
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 O      -4.955178    -0.902317    -0.169301     170.59
 H      -4.714773    -0.198203     0.518098      27.11
 C      -2.460843    -1.517918    -0.920968      66.33
 H      -1.801711    -1.750844    -1.888783      22.03
 C      -2.322822    -2.775598     0.151385      87.15
 O      -3.224249    -3.857040    -0.366053     262.65
 H      -3.138773    -4.120978    -1.181420      35.18
 H      -2.936526    -2.618376     1.175087      22.48
 H      -1.333368    -3.144531     0.331325      25.77
 C       1.858136    -0.538678    -1.016428      50.06
 H       2.748736    -1.181069    -1.496884      22.58
 C       1.425678     1.471240     0.553516      63.85
 H       2.118528     2.307075     1.095097      17.34
 C       0.036604     1.188610     0.437611       6.45
 O      -1.034792     1.719782     1.188166     205.80
 C      -0.589126     2.627127     2.223161     108.23
 H       0.129102     3.408195     1.789158      24.70
 H      -1.163469     3.293320     2.923719      23.80
 H       0.246526     1.991410     2.661519      25.42
 C      -0.433208    -0.041604    -0.305665     -19.75
 O      -1.745061    -0.469882    -0.206611     130.38
 C       0.536645    -0.944833    -0.957338      44.71
 H       0.158371    -2.096778    -1.223600      21.53
 C       2.308357     0.668591    -0.319893       9.70
 C       3.835446     0.856890    -0.214952      62.21
 H       4.055583     0.746185    -1.211685      25.29
 O       4.280456     2.365461     0.282207      90.18
 H       4.642897     2.392770     1.215185      25.71
 C       4.232914    -0.156577     1.015151      96.11
 H       3.973855     0.542871     1.802042      25.92
 O       3.632751    -1.412231     1.190308     262.18
 H       4.305780    -1.860993     1.792880      26.45
 C       5.741112    -0.431351     1.040196     108.15
 O       6.678459     0.769267     1.057052     258.70
 H       6.670696     0.980217     2.014983      28.13
 H       6.005813    -1.048944     0.276006      30.10
 H       6.107505    -0.935076     1.989745      27.75
55
name= lig-ACN-Water-frame_934
 C      -3.514609     0.463616    -3.569336      42.68
 H      -3.421412    -0.542027    -3.880904      24.48
 C      -3.875799     1.729056    -1.423788      38.42
 H      -4.193852     1.841599    -0.340186      21.00
 C      -4.192307     2.887861    -2.159932     -14.23
 O      -4.290626     4.174361    -1.563766     210.43
 C      -3.139717     4.684067    -0.856288     101.03
 H      -3.272241     5.890240    -0.295646      22.46
 H      -2.359289     4.778363    -1.647158      24.35
 H      -3.306115     4.087738     0.109864      24.06
 C      -4.141292     2.828062    -3.755835     -27.29
 O      -4.094154     3.957470    -4.545249     148.24
 H      -4.335703     4.889165    -4.143186      19.98
 C      -3.845671     1.590200    -4.439817      63.47
 H      -3.604263     1.385397    -5.533748      26.41
 C      -3.637173     0.438756    -2.126339      13.71
 C      -3.944117    -0.894411    -1.281612      83.08
 H      -4.247275    -1.627377    -1.938761      26.57
 O      -4.855254    -0.853353    -0.116951     232.22
 H      -4.679756    -0.095408     0.667669      21.84
 C      -2.456179    -1.481079    -0.947542      73.01
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 H      -2.043297    -1.725437    -2.045622      21.84
 C      -2.404980    -2.712589     0.052405      96.23
 O      -3.285413    -3.894371    -0.297409     245.42
 H      -2.873545    -3.875006    -1.192751      28.49
 H      -2.673060    -1.987807     0.959868      21.97
 H      -1.415607    -2.977535     0.248470      25.50
 C       1.941299    -0.507977    -0.888101       9.10
 H       2.773754    -1.054206    -1.549699      22.72
 C       1.392775     1.471005     0.409191      78.74
 H       1.645937     2.289935     1.231865      19.18
 C      -0.029705     1.110528     0.356038       0.95
 O      -1.005229     1.704864     1.127280     189.67
 C      -0.536425     2.589201     2.211418     101.46
 H       0.075031     3.379638     1.749788      24.93
 H      -1.651073     2.792244     2.377792      22.58
 H      -0.264428     2.132806     3.216308      25.20
 C      -0.392201    -0.107889    -0.338636      16.53
 O      -1.695525    -0.531591    -0.128972     152.57
 C       0.504519    -0.917752    -0.957448      53.33
 H       0.015352    -1.887569    -1.542885      21.25
 C       2.333902     0.710570    -0.267529      36.85
 C       3.838869     0.921253    -0.170159      75.19
 H       4.577210     0.618362    -0.801777      26.29
 O       4.203219     2.303223     0.311488     183.97
 H       4.803305     2.071507     1.063970      26.34
 C       4.229632    -0.165464     1.207993      66.92
 H       3.844301     0.296500     2.083255      25.79
 O       3.675999    -1.552355     1.191101     221.92
 H       4.149193    -2.196998     1.961529      25.60
 C       5.749557    -0.384507     1.068705     104.88
 O       6.660149     0.715288     1.085427     280.70
 H       7.041721     1.074821     1.880566      30.59
 H       5.878657    -0.934973     0.223553      31.51
 H       5.834631    -1.110070     1.976461      27.78
55
name= lig-ACN-Water-frame_935
 C      -3.478665     0.403589    -3.518514      56.39
 H      -3.406105    -0.513306    -4.125971      25.34
 C      -3.867817     1.687516    -1.419704      51.74
 H      -3.846828     1.718837    -0.358092      21.89
 C      -4.094841     2.893466    -2.277173      17.49
 O      -4.375997     4.155880    -1.663352     235.24
 C      -3.168100     4.553159    -0.842497      85.02
 H      -3.450476     5.845247    -0.817753      21.65
 H      -2.272329     4.300209    -1.212906      29.03
 H      -2.885166     3.996096     0.114847      25.22
 C      -4.117521     2.793517    -3.623020      -5.48
 O      -4.135203     3.921612    -4.584301     137.62
 H      -4.330421     4.838483    -4.125934      24.23
 C      -3.763655     1.536768    -4.319543       7.04
 H      -3.992579     1.691039    -5.410307      22.18
 C      -3.758979     0.444234    -2.035639       4.96
 C      -3.890882    -1.040741    -1.279535      96.31
 H      -4.493195    -1.719502    -1.826273      24.08
 O      -4.716455    -0.785345    -0.153686     267.03
 H      -4.057188    -0.335548     0.483856      24.08
 C      -2.504497    -1.469670    -0.921799      78.11
 H      -1.848619    -1.617576    -1.900790      20.47
 C      -2.559940    -2.649309    -0.041343     106.98
 O      -3.253734    -3.824616    -0.271836     206.83
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 H      -3.277317    -4.476648    -1.174042      26.37
 H      -2.931544    -2.650912     1.075000      21.77
 H      -1.585263    -2.949776    -0.048939      24.88
 C       1.929125    -0.475120    -0.899891      74.33
 H       2.623802    -1.259981    -1.365901      22.17
 C       1.264634     1.456137     0.282659      55.49
 H       1.467426     2.417452     0.799445      17.52
 C       0.022398     0.959929     0.316309      23.70
 O      -0.940171     1.637653     1.041403     199.92
 C      -0.666972     2.610315     2.219692     110.79
 H       0.012058     3.404420     1.977101      26.23
 H      -1.541506     3.317406     2.485944      24.57
 H      -0.244045     1.993453     3.090629      26.15
 C      -0.406132    -0.169337    -0.336564      24.71
 O      -1.726695    -0.497025    -0.052228     172.26
 C       0.673057    -0.829848    -0.994278      74.64
 H       0.616099    -1.757634    -1.695300      21.69
 C       2.356787     0.693423    -0.283352      49.13
 C       3.825277     0.845357     0.150175      94.03
 H       4.251489     0.511033    -0.754070      23.69
 O       4.111407     2.180000     0.325140     244.32
 H       4.997518     2.336347     0.686719      26.42
 C       4.237967    -0.085508     1.314160      82.29
 H       4.035310     0.297829     2.270649      24.15
 O       3.682728    -1.637540     1.146903     220.25
 H       4.304928    -2.019266     1.897978      26.29
 C       5.803472    -0.451275     1.227848     104.68
 O       6.688582     0.720042     1.058562     271.53
 H       6.732758     1.168540     1.952943      28.74
 H       5.858352    -0.806975     0.279054      30.15
 H       6.464887    -1.226567     1.847458      27.53
55
name= lig-ACN-Water-frame_936
 C      -3.620878     0.346034    -3.430265      48.31
 H      -3.264735    -0.605327    -3.943981      21.56
 C      -3.942040     1.669337    -1.525124      53.48
 H      -3.828790     1.818314    -0.537045      21.92
 C      -4.011095     2.843376    -2.243742     -34.31
 O      -4.372005     4.079287    -1.735877     312.65
 C      -3.238088     4.437918    -0.832659      91.91
 H      -3.079569     5.790179    -0.778744      22.49
 H      -2.444726     4.120460    -1.389312      25.61
 H      -3.580605     4.219093     0.160822      26.95
 C      -3.935422     2.817778    -3.694129      49.74
 O      -4.218868     3.797994    -4.546740     195.01
 H      -4.381415     4.618539    -4.077837      23.64
 C      -3.737329     1.574908    -4.100922      61.25
 H      -3.620019     1.320631    -5.183283      25.91
 C      -3.816050     0.356492    -2.143469      41.30
 C      -3.846326    -0.820170    -1.354308     119.82
 H      -4.192474    -1.630367    -2.023986      26.63
 O      -4.593536    -0.742928    -0.115091     281.61
 H      -4.171309    -0.374535     0.607500      28.21
 C      -2.480839    -1.478636    -0.910993      82.05
 H      -1.818910    -1.748435    -1.820609      20.72
 C      -2.468560    -2.777296     0.041937      88.29
 O      -3.386741    -3.901411    -0.327724     200.70
 H      -2.883588    -3.991930    -1.445991      23.09
 H      -2.863727    -2.142330     0.922108      21.68
 H      -1.515632    -3.004626     0.254611      25.46
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 C       2.106771    -0.454576    -0.991906      36.60
 H       2.981688    -1.067908    -1.195859      17.70
 C       1.351783     1.525126     0.198458      37.91
 H       1.632602     2.452551     0.509732      17.09
 C       0.003672     0.990520     0.383991      -0.47
 O      -1.006144     1.647788     1.024866     197.04
 C      -0.714649     2.628930     2.176757      93.32
 H       0.151477     3.156277     1.864040      23.67
 H      -1.756840     2.989822     2.427592      21.72
 H      -0.502251     1.866403     2.987416      23.94
 C      -0.423189    -0.265315    -0.331244      -7.24
 O      -1.819695    -0.500834    -0.064208     194.55
 C       0.583744    -0.932119    -1.119870      51.53
 H       0.248720    -1.939208    -1.461359      18.57
 C       2.371001     0.641109    -0.168659      35.40
 C       3.780905     0.626121     0.261192      73.58
 H       4.437218     0.217070    -0.482633      22.12
 O       4.063051     2.197075     0.414453     245.33
 H       5.035607     2.258599     0.190162      25.69
 C       4.344864    -0.240367     1.472559      95.10
 H       3.904373     0.145122     2.364260      22.01
 O       3.731261    -1.535941     1.152879     353.19
 H       4.123036    -2.178476     1.669794      29.83
 C       5.868840    -0.466242     1.202330      85.20
 O       6.713447     0.757420     1.051338     329.58
 H       7.012926     1.184163     1.992362      25.61
 H       5.932788    -1.132650     0.395172      31.67
 H       6.029371    -1.017454     2.280792      24.93
55
name= lig-ACN-Water-frame_937
 C      -3.718409     0.292745    -3.528372      48.58
 H      -3.627711    -0.776664    -4.010039      22.90
 C      -4.011291     1.668947    -1.516830      79.48
 H      -4.300606     1.621889    -0.528159      20.98
 C      -4.050771     2.830190    -2.309142      21.03
 O      -4.319345     4.052583    -1.742826     293.14
 C      -3.342780     4.415397    -0.802749      96.45
 H      -3.111699     5.734714    -0.936108      21.55
 H      -2.465471     3.903389    -0.671194      29.08
 H      -3.614466     4.157861     0.195647      25.65
 C      -3.795884     2.765483    -3.635886     -16.85
 O      -4.309343     3.761491    -4.543804     200.00
 H      -4.241894     4.664874    -4.231149      21.59
 C      -3.608650     1.408075    -4.309450       9.98
 H      -3.256110     1.528414    -5.338441      25.92
 C      -3.820762     0.446471    -2.052644      20.43
 C      -3.789859    -0.894817    -1.220975     113.62
 H      -4.491578    -1.569901    -1.816456      25.23
 O      -4.581255    -0.707970    -0.062030     301.79
 H      -4.052996    -0.262587     0.513069      28.91
 C      -2.341423    -1.576613    -0.927410      72.30
 H      -1.905064    -1.694130    -1.952826      19.44
 C      -2.491514    -2.813130     0.142205      96.36
 O      -3.411808    -3.915364    -0.441593     237.78
 H      -3.241031    -4.050728    -1.587529      26.59
 H      -2.976738    -2.650436     1.140993      21.99
 H      -1.619800    -3.268364     0.283862      24.61
 C       1.927127    -0.596068    -1.058700      35.54
 H       2.589462    -1.201163    -1.580127      20.16
 C       1.329623     1.543577     0.277689      47.53
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 H       1.526485     2.365618     0.784747      17.67
 C       0.037916     1.040018     0.328416      -1.57
 O      -1.121468     1.688222     1.009432     227.51
 C      -0.728579     2.514451     2.126189     128.54
 H      -0.150766     3.427840     1.917293      23.81
 H      -1.581285     3.222472     2.191356      24.63
 H      -0.533666     2.145941     3.117326      25.57
 C      -0.322964    -0.215854    -0.278708      -6.29
 O      -1.721455    -0.515553    -0.169452     217.46
 C       0.583967    -0.973338    -1.097687      61.81
 H       0.376502    -1.851700    -1.624072      19.72
 C       2.374553     0.438240    -0.155324      35.76
 C       3.874760     0.696239     0.292124      77.97
 H       4.475000     0.455915    -0.604652      19.71
 O       4.069730     2.097674     0.493756     266.39
 H       5.034819     2.187918     0.198343      24.21
 C       4.371295    -0.299725     1.492588     104.21
 H       4.405669    -0.040268     2.567956      20.96
 O       3.752172    -1.505379     1.182186     300.13
 H       4.122830    -2.236976     1.789218      26.59
 C       5.933498    -0.409933     1.361689      98.24
 O       6.720603     0.706438     0.984037     298.19
 H       7.018969     1.284185     1.901003      23.60
 H       6.209115    -1.096888     0.567417      30.07
 H       6.553736    -0.930580     2.321424      26.42
55
name= lig-ACN-Water-frame_938
 C      -3.710884     0.250673    -3.556649      36.15
 H      -3.892035    -0.815093    -3.992508      20.97
 C      -4.096623     1.673450    -1.420799      33.82
 H      -4.421892     1.877105    -0.382323      19.65
 C      -4.073693     2.775590    -2.310518     -17.82
 O      -4.304610     4.075995    -1.778866     191.13
 C      -3.392007     4.428365    -0.574816      85.51
 H      -3.038226     5.690462    -1.021357      22.02
 H      -2.506306     3.878682    -0.825914      23.17
 H      -3.957972     4.621345     0.206488      25.03
 C      -3.802824     2.593022    -3.840645      -8.00
 O      -4.309676     3.724641    -4.557718     152.18
 H      -4.188996     4.575415    -3.975977      22.57
 C      -3.465874     1.436024    -4.484162      75.56
 H      -3.542361     1.331053    -5.557385      23.58
 C      -3.779127     0.334024    -2.130677       0.36
 C      -3.818241    -1.044804    -1.128606      77.35
 H      -4.319075    -1.940295    -1.708274      23.31
 O      -4.577337    -0.666338     0.066984     284.16
 H      -4.054013    -0.431996     0.762981      27.37
 C      -2.367970    -1.628070    -0.834117     102.35
 H      -1.802149    -2.172220    -1.578735      20.37
 C      -2.563930    -2.943840     0.015777     116.91
 O      -3.400520    -3.857950    -0.523729     337.42
 H      -3.139636    -4.043709    -1.441766      34.47
 H      -3.005659    -2.601464     0.943276      24.98
 H      -1.619660    -3.224552     0.196403      27.04
 C       1.897176    -0.690424    -0.997392      52.49
 H       2.481468    -1.209585    -1.655370      22.76
 C       1.412685     1.265726     0.414779      69.74
 H       1.865759     2.003836     0.990455      21.94
 C      -0.044464     1.060057     0.301841      25.13
 O      -1.090392     1.680697     0.950701     236.34
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 C      -0.817332     2.625516     2.090535      95.83
 H       0.150241     3.003523     1.787618      22.38
 H      -1.718489     3.052148     2.465829      23.91
 H      -0.427961     1.873052     2.738528      25.03
 C      -0.340927    -0.164806    -0.308145      28.24
 O      -1.548497    -0.520928    -0.274637     211.45
 C       0.515136    -0.971898    -1.013363      53.13
 H       0.037524    -1.664132    -1.557288      19.28
 C       2.315012     0.470711    -0.164972      39.07
 C       3.901587     0.671755     0.243163      82.34
 H       4.447132     0.312070    -0.668243      22.73
 O       4.113693     2.054814     0.591837     248.87
 H       5.022566     2.363783     0.718236      25.45
 C       4.497939    -0.172390     1.451066      76.30
 H       3.792992     0.325085     2.188020      22.24
 O       3.749043    -1.612925     1.228492     202.31
 H       4.254455    -2.116846     2.085481      25.76
 C       6.072527    -0.493806     1.455745      85.23
 O       6.756683     0.723761     0.889273     238.01
 H       6.908812     1.393828     1.792051      21.81
 H       6.060072    -1.327713     0.716286      29.08
 H       6.472175    -0.827497     2.594369      25.46
55
name= lig-ACN-Water-frame_939
 C      -3.580400     0.244947    -3.527336      41.36
 H      -3.427934    -0.753268    -4.051713      23.83
 C      -4.072157     1.509584    -1.604107      58.42
 H      -4.018297     1.582824    -0.440771      19.80
 C      -4.035479     2.667087    -2.374323       0.24
 O      -4.271257     4.066325    -1.823075     199.51
 C      -3.476962     4.508626    -0.563666      66.23
 H      -2.816102     5.685670    -0.703192      21.06
 H      -2.789902     3.760628    -0.108411      25.55
 H      -4.035558     4.426827     0.252176      25.46
 C      -3.953485     2.618000    -3.832351      -3.48
 O      -4.219571     3.682636    -4.589632     155.46
 H      -4.539488     4.437387    -3.910220      20.88
 C      -3.526409     1.334359    -4.421648      56.00
 H      -3.625661     1.108774    -5.454817      23.06
 C      -3.840174     0.225494    -2.105119      35.33
 C      -3.822081    -0.986620    -1.163771      90.80
 H      -4.506431    -1.865214    -1.568695      22.60
 O      -4.581370    -0.723514     0.131893     259.76
 H      -4.133646    -0.194861     0.741516      27.01
 C      -2.432060    -1.662001    -0.841038      92.01
 H      -2.219204    -1.672920    -1.880624      21.56
 C      -2.500145    -2.903252     0.091037     111.58
 O      -3.434698    -3.882270    -0.672253     303.46
 H      -3.141720    -4.116884    -1.463336      34.92
 H      -2.947408    -2.707159     1.010832      25.71
 H      -1.653408    -3.428277     0.267691      26.34
 C       2.002299    -0.687912    -0.925688      46.68
 H       2.826958    -1.267190    -1.264024      22.75
 C       1.393115     1.104269     0.656323      53.59
 H       1.704331     1.894541     1.409477      19.66
 C       0.042467     1.044966     0.361215       7.92
 O      -1.100744     1.733884     0.876557     201.71
 C      -0.721217     2.580359     2.045876     134.46
 H      -0.330400     3.636693     1.941268      23.73
 H      -1.641296     3.024368     2.234977      26.94
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 H      -0.555806     2.072084     2.963483      26.74
 C      -0.350809    -0.141748    -0.404935     -11.45
 O      -1.778331    -0.566345    -0.260249     145.09
 C       0.579154    -0.987798    -1.011438      68.67
 H       0.288691    -1.911606    -1.425462      22.05
 C       2.457613     0.367557    -0.190928      25.29
 C       3.912272     0.541692     0.076822      75.52
 H       4.638556     0.529995    -0.801953      23.55
 O       4.129230     2.100911     0.674348      97.39
 H       4.994888     1.804115     1.012981      23.59
 C       4.395357    -0.245072     1.342340      96.26
 H       4.329813     0.255378     2.385247      19.79
 O       3.870366    -1.619463     1.351465     270.07
 H       4.044068    -2.201725     2.182478      26.11
 C       5.992654    -0.440210     1.446503      90.97
 O       6.803127     0.689295     0.838402     157.93
 H       7.279791     1.214745     1.702559      26.46
 H       6.481836    -1.396955     0.952504      28.30
 H       6.306471    -0.567169     2.636399      26.29
55
name= lig-ACN-Water-frame_940
 C      -3.408595     0.060450    -3.493779      76.61
 H      -2.892267    -0.775814    -3.948666      27.55
 C      -3.968454     1.458198    -1.687223      51.50
 H      -4.093067     1.599480    -0.494420      21.08
 C      -4.015017     2.710837    -2.376833      15.02
 O      -4.160768     3.970413    -1.849030     263.02
 C      -3.640279     4.422383    -0.577536      87.26
 H      -3.048330     5.630328    -0.861738      21.26
 H      -2.772221     3.687112    -0.297854      21.82
 H      -4.380637     4.786023    -0.102328      25.02
 C      -4.035996     2.546706    -3.749630      -3.38
 O      -4.131307     3.699534    -4.656038     191.43
 H      -4.497909     4.535781    -4.287340      22.97
 C      -3.760564     1.278980    -4.238084      49.87
 H      -3.272160     1.386118    -5.185135      24.16
 C      -3.848653     0.146484    -2.169961      28.75
 C      -3.985392    -0.990637    -1.114296      95.25
 H      -4.668889    -1.692414    -1.759963      19.56
 O      -4.602413    -0.819451     0.097434     265.60
 H      -4.129578    -0.102762     0.685063      21.98
 C      -2.546306    -1.598722    -0.985104      79.66
 H      -1.888940    -1.998257    -1.686592      18.11
 C      -2.525773    -2.947678     0.008358     103.33
 O      -3.449057    -3.882134    -0.696533     262.07
 H      -2.993038    -3.859548    -1.619458      28.61
 H      -2.977232    -2.744219     0.881473      23.99
 H      -1.511068    -3.214118     0.081394      23.20
 C       2.058582    -0.716546    -0.912951      52.26
 H       2.610892    -1.582189    -1.350724      19.97
 C       1.492828     1.040040     0.771234      59.56
 H       1.768173     1.829358     1.636569      14.84
 C       0.038099     0.840288     0.380829      -1.62
 O      -0.931986     1.788368     0.852376     192.15
 C      -0.818926     2.652018     2.031084      99.92
 H       0.004470     3.332944     1.609216      21.59
 H      -1.780913     2.823518     2.340242      24.56
 H      -0.192425     2.138233     2.821004      25.14
 C      -0.470061    -0.244642    -0.469963      12.17
 O      -1.829554    -0.453993    -0.163084     163.78
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 C       0.699868    -1.032003    -1.011843      51.59
 H       0.513318    -2.055839    -1.427151      18.56
 C       2.426322     0.377269    -0.009770      29.55
 C       3.937078     0.644699     0.147868      76.67
 H       4.426381     0.440285    -0.903476      21.31
 O       4.159733     1.974831     0.659218     194.64
 H       4.942526     2.198029     1.223409      24.16
 C       4.465582    -0.374480     1.276208      96.57
 H       3.800754     0.264167     2.040908      18.90
 O       3.942952    -1.656734     1.459610     288.01
 H       4.286358    -1.854721     2.263889      26.71
 C       5.954590    -0.349330     1.387001      93.28
 O       6.837960     0.631910     0.813622     225.73
 H       6.930905     1.326176     1.645193      26.83
 H       6.236237    -1.496912     1.004659      27.40
 H       6.132089    -0.265329     2.569825      23.92
55
name= lig-ACN-Water-frame_941
 C      -3.391458     0.004726    -3.510582      53.40
 H      -3.010162    -0.861528    -3.967314      24.62
 C      -3.946194     1.516499    -1.546198      57.12
 H      -4.289179     1.586687    -0.407169      20.15
 C      -4.019773     2.643667    -2.335566      15.76
 O      -4.098698     3.924947    -1.908518     258.66
 C      -3.760809     4.382531    -0.634810      87.65
 H      -2.944731     5.388338    -0.995823      20.17
 H      -3.213553     3.662965     0.150416      21.15
 H      -4.477213     4.509361     0.016812      23.03
 C      -4.088421     2.572359    -3.766709      -7.04
 O      -4.041212     3.607439    -4.712183     249.21
 H      -4.030535     4.386418    -4.180371      26.33
 C      -3.764227     1.196080    -4.241692      32.38
 H      -3.488938     1.187432    -5.318963      23.10
 C      -3.799604     0.166407    -2.133484      11.97
 C      -4.034000    -1.102275    -1.295118      77.63
 H      -4.615361    -2.027660    -1.626143      21.66
 O      -4.681076    -0.875466     0.098520     207.90
 H      -3.905596    -0.322873     0.719959      17.04
 C      -2.577975    -1.587284    -0.884441      84.57
 H      -2.211483    -1.531588    -1.877104      16.63
 C      -2.621472    -2.857275    -0.171707     123.55
 O      -3.412830    -3.887528    -0.664384     275.40
 H      -3.472695    -4.199496    -1.757882      25.80
 H      -2.862846    -2.719005     0.803620      24.29
 H      -1.646949    -3.323113    -0.096323      22.84
 C       2.004598    -0.673897    -0.805846      45.53
 H       2.981811    -0.983084    -1.373635      18.79
 C       1.381770     0.963179     0.727835      68.21
 H       1.797298     1.885516     1.438084      14.83
 C       0.109620     0.764221     0.501590      21.71
 O      -0.799473     1.717467     0.794285     225.45
 C      -0.731591     2.672194     1.963823     115.10
 H      -0.490056     3.831144     1.842067      22.00
 H      -1.701140     2.906470     2.338221      23.83
 H      -0.286674     2.076023     2.839950      24.09
 C      -0.353497    -0.293332    -0.321397      17.69
 O      -1.803913    -0.453643    -0.206839     176.60
 C       0.583550    -1.104852    -0.981386      70.80
 H       0.211074    -1.971851    -1.696990      16.28
 C       2.449460     0.291128     0.081528      53.84
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 C       3.913672     0.601781     0.213285      85.34
 H       4.437370     0.510952    -0.848620      19.21
 O       4.156336     1.948750     0.603670     207.41
 H       4.924535     1.871554     1.199247      24.25
 C       4.468780    -0.196785     1.302445     106.23
 H       4.201305     0.222187     2.376920      18.04
 O       3.987881    -1.790576     1.493818     183.59
 H       4.336249    -2.151960     2.343891      25.37
 C       6.004023    -0.393120     1.455043      98.17
 O       6.803128     0.666604     0.777461     150.15
 H       7.115399     1.345171     1.506098      30.09
 H       6.360460    -1.430441     0.793039      28.31
 H       6.328953    -0.575695     2.553161      29.32
55
name= lig-ACN-Water-frame_942
 C      -3.589849     0.163212    -3.458139      78.49
 H      -3.664996    -0.792204    -3.863766      24.42
 C      -4.012434     1.396748    -1.444040      57.59
 H      -4.074304     1.498085    -0.314424      18.40
 C      -4.043446     2.555416    -2.392152     -21.24
 O      -4.104815     3.974666    -1.997379     215.00
 C      -3.794290     4.343296    -0.558995      69.19
 H      -3.152904     5.461447    -0.238058      21.22
 H      -3.223415     3.376878    -0.193188      22.81
 H      -4.674827     4.598129    -0.226949      25.42
 C      -3.973001     2.348750    -3.825715      -7.72
 O      -3.978090     3.484295    -4.686551     189.20
 H      -3.899320     4.381345    -4.208200      23.58
 C      -3.623733     1.180004    -4.419018      61.19
 H      -3.936169     0.933272    -5.465053      19.91
 C      -3.805098     0.210052    -2.036086      26.30
 C      -3.953298    -1.078039    -1.191624     103.39
 H      -4.421290    -1.730392    -1.945049      23.30
 O      -4.757866    -0.922810     0.012663     266.53
 H      -4.079104    -0.438442     0.698687      22.23
 C      -2.529644    -1.473670    -1.033876      89.79
 H      -2.002038    -1.796122    -1.925700      18.07
 C      -2.513363    -2.870745    -0.167471      87.96
 O      -3.508488    -3.986435    -0.647976     181.76
 H      -3.190823    -3.932005    -1.816898      23.80
 H      -2.924709    -2.609735     0.762192      22.95
 H      -1.429318    -3.161083    -0.229225      20.07
 C       1.901387    -0.784983    -0.839662      47.36
 H       2.473278    -1.288611    -1.750006      19.71
 C       1.515810     1.018005     0.806826      53.67
 H       1.648258     2.123587     1.298796      12.90
 C       0.095888     0.758899     0.592620       4.63
 O      -0.829268     1.751888     0.803332     215.44
 C      -0.684726     2.629162     1.921376      87.57
 H      -0.191361     3.574968     1.363325      19.37
 H      -1.720292     2.587673     2.103877      22.40
 H      -0.032576     2.391092     2.914820      23.45
 C      -0.377344    -0.430717    -0.104722      11.71
 O      -1.769263    -0.529345    -0.262170     220.25
 C       0.597869    -1.079607    -0.927847      57.99
 H       0.223785    -1.910182    -1.773487      15.60
 C       2.380496     0.187507     0.098803      38.83
 C       3.853244     0.493450     0.206219      49.56
 H       4.485252     0.060081    -0.690243      22.60
 O       4.136604     2.034568     0.553620     148.58
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 H       4.931857     2.052408     1.123138      26.46
 C       4.563320    -0.362091     1.634520      74.54
 H       4.181777     0.321603     2.496821      22.76
 O       4.040698    -1.754885     1.436941     207.38
 H       4.360263    -2.215401     2.407692      24.33
 C       6.096728    -0.475048     1.427311      77.57
 O       6.768104     0.737639     0.781385     103.55
 H       6.973448     1.288653     1.566068      28.06
 H       6.315826    -1.475330     0.598971      28.72
 H       6.585641    -0.651582     2.398435      31.06
55
name= lig-ACN-Water-frame_943
 C      -3.844785     0.051723    -3.441132      45.35
 H      -3.933642    -0.968329    -3.739022      23.88
 C      -4.062497     1.564796    -1.463452      72.78
 H      -4.046079     1.719742    -0.433144      16.72
 C      -4.032055     2.584617    -2.345384       5.00
 O      -4.086282     3.965065    -2.067215     237.94
 C      -3.880159     4.218152    -0.555297      78.46
 H      -3.075900     5.164987    -0.788052      21.73
 H      -3.292457     3.427716     0.082237      24.25
 H      -4.690797     4.271147     0.124372      24.28
 C      -3.761341     2.369382    -3.844327      -9.38
 O      -3.940100     3.412613    -4.651323     193.91
 H      -4.202853     4.199359    -3.989972      22.93
 C      -3.626047     1.075344    -4.447844      51.29
 H      -3.462732     0.908257    -5.586837      21.94
 C      -3.886265     0.256664    -2.049035      50.52
 C      -3.867090    -0.951576    -1.214828     122.67
 H      -4.376326    -1.790017    -1.673575      26.23
 O      -4.769671    -0.985123    -0.085778     285.16
 H      -4.499957    -0.513215     0.631754      30.58
 C      -2.374417    -1.661145    -1.078271      66.77
 H      -1.965341    -1.693359    -2.117529      21.50
 C      -2.464812    -2.954670    -0.171598      97.29
 O      -3.469709    -3.953112    -0.643114     182.04
 H      -3.207512    -4.211317    -1.732176      25.76
 H      -2.695168    -2.663034     0.893746      24.40
 H      -1.458642    -3.535272    -0.010979      22.82
 C       1.934176    -0.875881    -0.890738      25.93
 H       2.698799    -1.570244    -1.467244      21.63
 C       1.480668     1.004890     0.819917      51.95
 H       2.207314     1.763706     1.301709      15.75
 C       0.107284     0.739506     0.635267       0.06
 O      -0.880597     1.678628     0.828314     208.34
 C      -0.704584     2.702849     1.881403      93.55
 H      -0.254506     3.758727     1.488073      21.74
 H      -1.351698     3.192672     2.528273      25.21
 H       0.083795     2.076565     2.564806      22.78
 C      -0.402741    -0.481017     0.023227      14.86
 O      -1.757611    -0.556996    -0.256878     176.41
 C       0.463964    -1.111840    -0.840331      47.64
 H       0.028502    -1.984689    -1.618189      18.20
 C       2.423529     0.167300     0.091815      -7.75
 C       3.958750     0.426808     0.464052      73.43
 H       4.515978     0.153264    -0.518632      23.22
 O       4.055188     1.961278     0.425240     202.71
 H       4.898557     2.222877     0.872718      23.66
 C       4.601365    -0.459336     1.646851     105.64
 H       4.247081    -0.180676     2.656341      24.47
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 O       4.100436    -1.689472     1.451073     266.91
 H       4.092014    -2.397740     2.240190      26.79
 C       6.196121    -0.479853     1.386732      75.41
 O       6.716969     0.727526     0.830712     221.13
 H       6.811736     1.473253     1.455718      23.97
 H       6.227009    -1.406993     0.415708      27.71
 H       6.810057    -0.872493     2.168361      30.53
55
name= lig-ACN-Water-frame_944
 C      -4.007774    -0.105413    -3.502844      50.36
 H      -3.857883    -1.151280    -3.848077      19.38
 C      -4.030131     1.620929    -1.548797      68.18
 H      -4.165601     1.712416    -0.571600      21.01
 C      -3.944818     2.668070    -2.509528      19.78
 O      -4.098532     3.912426    -1.993303     263.03
 C      -3.872948     4.146058    -0.668906      98.32
 H      -3.435742     5.343178    -0.461870      21.16
 H      -3.106863     3.407697    -0.355872      25.92
 H      -4.895964     4.340100    -0.288379      22.21
 C      -3.658036     2.352470    -3.756200      27.01
 O      -3.897183     3.495082    -4.668653     206.25
 H      -4.114086     4.329690    -4.185879      26.30
 C      -3.699315     0.994373    -4.234225      68.59
 H      -3.200398     0.926209    -5.254262      25.46
 C      -4.025004     0.306562    -2.088212      10.38
 C      -3.845446    -1.115623    -1.299775      90.76
 H      -4.249652    -1.715369    -2.052840      28.75
 O      -4.735032    -1.041378    -0.102556     279.73
 H      -4.240750    -0.435853     0.442025      27.71
 C      -2.356880    -1.695720    -0.931662      82.09
 H      -1.852017    -1.825485    -1.945750      19.91
 C      -2.400745    -3.070620    -0.205636     109.51
 O      -3.416279    -3.900593    -0.629631     287.19
 H      -3.256457    -4.153594    -1.488177      34.96
 H      -2.869139    -2.707003     0.817531      22.93
 H      -1.324113    -3.596471    -0.174808      22.35
 C       1.928708    -0.867855    -0.712904      62.96
 H       2.724058    -1.481602    -1.216564      21.76
 C       1.492880     0.863102     0.742697      67.72
 H       1.554319     1.664317     1.437087      18.72
 C       0.075509     0.739368     0.666859       8.26
 O      -1.033703     1.650372     0.939088     188.86
 C      -0.572138     2.785490     1.885580      97.71
 H      -0.092105     3.575333     1.110804      20.81
 H      -1.562372     2.763049     2.165620      22.43
 H       0.210654     2.468143     2.807394      23.54
 C      -0.361176    -0.397521    -0.043807       4.22
 O      -1.757352    -0.598319    -0.186716     169.37
 C       0.581105    -1.236288    -0.779589      63.83
 H       0.031754    -2.110610    -1.396184      16.69
 C       2.485082     0.061129     0.108686      43.79
 C       3.962744     0.409970     0.501363      87.99
 H       4.661072    -0.038829    -0.310260      22.60
 O       3.980718     1.818890     0.352987     255.58
 H       4.873192     2.108184     0.621030      25.37
 C       4.708115    -0.345044     1.643122      95.36
 H       4.705261     0.074432     2.613059      25.29
 O       4.081629    -1.842513     1.424735     246.44
 H       4.230408    -2.037273     2.310887      27.12
 C       6.175360    -0.533121     1.342096      85.56
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 O       6.696525     0.735867     0.829356     220.96
 H       7.084886     1.109026     1.690105      26.50
 H       6.400084    -1.278057     0.268642      26.25
 H       6.671767    -0.907139     2.170659      30.94
55
name= lig-ACN-Water-frame_945
 C      -4.023888    -0.049956    -3.417935      40.20
 H      -4.027800    -1.080208    -3.929472      21.40
 C      -4.009331     1.400525    -1.663653      67.71
 H      -4.107843     1.634794    -0.660642      20.47
 C      -3.861479     2.628868    -2.386354      -5.55
 O      -4.113053     3.976843    -2.098989     269.43
 C      -3.863342     4.204748    -0.647018      82.68
 H      -3.460567     5.364790    -0.555078      22.32
 H      -3.120680     3.568670    -0.153335      26.38
 H      -4.635467     3.773784     0.034209      23.82
 C      -3.743713     2.447597    -3.887521      -6.35
 O      -3.781974     3.519085    -4.730595     214.86
 H      -3.772766     4.240419    -4.124006      25.78
 C      -3.693831     1.093502    -4.271317      69.17
 H      -3.734559     0.805775    -5.349901      24.71
 C      -4.083242     0.018266    -2.085512      46.90
 C      -3.922219    -1.204758    -1.304053     114.22
 H      -4.300255    -2.076432    -1.710283      24.78
 O      -4.627173    -1.131428    -0.110435     250.52
 H      -4.099930    -0.575939     0.700523      21.30
 C      -2.417316    -1.597999    -0.924098      71.94
 H      -1.718082    -1.784531    -1.789371      20.47
 C      -2.351828    -3.020685    -0.091559      90.43
 O      -3.433260    -3.942817    -0.677514     283.71
 H      -3.352395    -4.044248    -1.598112      33.64
 H      -2.327495    -3.045664     1.127204      22.39
 H      -1.243241    -3.453890    -0.340075      19.70
 C       2.056563    -1.036192    -0.586380      33.36
 H       2.571340    -1.561672    -1.339574      21.89
 C       1.402732     0.901207     0.840952      58.98
 H       1.901594     1.634664     1.304601      19.76
 C      -0.015062     0.684433     0.549549      -2.69
 O      -0.969245     1.574732     1.147465     192.18
 C      -0.577725     2.801228     1.817389     104.60
 H      -0.110204     3.660740     1.104107      22.70
 H      -1.208120     3.581467     2.252306      24.81
 H       0.108128     2.655524     2.828771      23.23
 C      -0.402883    -0.444107    -0.267233      26.43
 O      -1.724668    -0.645551    -0.058794     219.46
 C       0.640827    -1.272657    -0.664199      62.01
 H       0.566877    -2.161444    -1.316222      19.76
 C       2.413610     0.049234     0.310792      18.15
 C       3.919532     0.285988     0.270131      72.65
 H       4.265560    -0.124034    -0.735611      22.46
 O       3.983536     1.762252     0.357795     247.44
 H       4.932409     1.991548     0.321420      24.46
 C       4.668889    -0.402235     1.567816      95.14
 H       4.330176    -0.010776     2.449199      25.28
 O       4.131198    -1.849535     1.527050     281.96
 H       4.198796    -2.416977     2.268488      29.29
 C       6.166014    -0.581140     1.244246      81.36
 O       6.750119     0.735385     0.835194     230.31
 H       6.884180     1.498844     1.584193      21.37
 H       6.184554    -1.619041     0.428039      25.02
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 H       6.716644    -0.896702     2.056689      29.49
55
name= lig-ACN-Water-frame_946
 C      -3.914785     0.030507    -3.605541      68.39
 H      -4.194955    -0.934931    -4.180365      26.88
 C      -4.005041     1.259835    -1.547493      30.60
 H      -3.991020     1.299072    -0.441265      16.38
 C      -3.876431     2.484273    -2.512856     -31.15
 O      -4.058703     3.930160    -2.098810     211.55
 C      -3.796541     4.279005    -0.630665     100.38
 H      -3.869720     5.514784    -0.572400      23.55
 H      -2.798017     4.013646    -0.523765      25.57
 H      -4.881255     4.136779    -0.135264      23.68
 C      -3.847159     2.437300    -3.865047      -6.19
 O      -3.636265     3.540378    -4.770469     141.78
 H      -3.859676     4.393239    -4.258766      22.90
 C      -3.821377     1.133951    -4.451413      54.01
 H      -3.936392     1.097727    -5.519159      14.53
 C      -4.038700    -0.025772    -2.135069      15.55
 C      -3.897519    -1.336397    -1.171819     102.80
 H      -4.274225    -2.089245    -1.786912      24.98
 O      -4.619245    -1.221117     0.065064     231.25
 H      -4.003806    -0.680668     0.811574      20.59
 C      -2.437406    -1.659342    -0.891612      86.53
 H      -2.065112    -1.549468    -1.946669      21.95
 C      -2.398286    -2.983513    -0.201958      93.31
 O      -3.367691    -3.956293    -0.659192     193.09
 H      -3.136962    -3.927238    -1.754629      25.58
 H      -2.726037    -2.897872     0.977397      21.41
 H      -1.333880    -3.559218    -0.423910      19.98
 C       2.014455    -1.127842    -0.415910      91.86
 H       2.909942    -1.372850    -0.805373      27.76
 C       1.372428     0.915100     0.901438      66.89
 H       1.503752     1.721585     1.483692      20.34
 C       0.063513     0.790322     0.548489      -7.94
 O      -0.926782     1.440767     1.320801     193.34
 C      -0.506516     2.888777     1.758621      69.63
 H       0.153464     3.190521     0.880903      24.23
 H      -1.631125     3.116463     2.004322      20.73
 H       0.244761     2.549382     2.618536      22.01
 C      -0.373252    -0.395543    -0.230491     -30.11
 O      -1.784939    -0.701644    -0.009565     145.45
 C       0.645323    -1.396949    -0.707934      65.05
 H       0.159220    -2.158769    -1.168165      22.28
 C       2.330416    -0.033050     0.335128      30.60
 C       3.813925     0.243458     0.215590      85.75
 H       4.247992    -0.005188    -0.765008      27.22
 O       4.064795     1.694853     0.364740     252.94
 H       4.987841     1.867798     0.047887      27.09
 C       4.532472    -0.570752     1.352049     103.24
 H       4.350057     0.105902     2.123643      28.07
 O       4.169476    -1.858318     1.607356     242.10
 H       4.551816    -1.828746     2.617801      24.39
 C       6.151522    -0.532973     1.265859      87.47
 O       6.789966     0.684304     0.801863     123.74
 H       6.849849     1.252385     1.661818      22.76
 H       6.443950    -1.037731     0.110979      26.65
 H       6.667870    -1.045279     2.058580      32.33
55
name= lig-ACN-Water-frame_947
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 C      -3.892626    -0.063756    -3.764155      74.07
 H      -3.757774    -1.101333    -4.253710      24.31
 C      -3.972330     1.340477    -1.601366      66.94
 H      -3.940058     1.521615    -0.439793      17.15
 C      -4.007097     2.462362    -2.356919       4.21
 O      -3.964015     3.745309    -2.023292     302.03
 C      -3.784136     4.392986    -0.781132      72.69
 H      -3.866498     5.556703    -0.963126      20.35
 H      -2.910872     4.242249    -0.228536      30.37
 H      -4.305924     3.772901     0.039403      23.85
 C      -3.848187     2.387468    -3.940245     -17.56
 O      -3.554383     3.531378    -4.718207     201.52
 H      -3.884870     4.383972    -4.161796      20.29
 C      -4.017615     1.173104    -4.577806      51.51
 H      -3.776818     1.067774    -5.590825      24.67
 C      -3.902600     0.086090    -2.280836       9.48
 C      -3.932917    -1.296977    -1.118473      70.71
 H      -4.457972    -2.125896    -1.577539      21.66
 O      -4.656752    -1.298009     0.253225     235.98
 H      -4.214394    -0.640711     0.787029      25.58
 C      -2.427463    -1.701417    -0.965359      65.79
 H      -1.786349    -1.785136    -1.891306      18.72
 C      -2.379746    -3.063628    -0.276362      98.78
 O      -3.315834    -3.997321    -0.699190     171.55
 H      -3.298894    -4.400323    -1.807599      23.75
 H      -2.751840    -2.663634     0.775364      21.46
 H      -1.280440    -3.364825     0.129732      22.71
 C       1.812184    -1.183695    -0.329762      13.26
 H       2.475295    -1.997379    -0.642768      22.70
 C       1.464416     0.919501     0.891486      65.76
 H       1.950644     1.555579     1.606443      18.54
 C       0.015702     0.704195     0.645028      17.14
 O      -0.889243     1.336305     1.395456     215.10
 C      -0.445908     2.760645     1.707002     114.41
 H      -0.172050     3.402323     0.862655      24.12
 H      -1.476922     3.447824     1.746497      20.50
 H      -0.128741     3.270086     2.653281      23.84
 C      -0.359521    -0.431692    -0.063084      13.62
 O      -1.757372    -0.700748    -0.027715     162.99
 C       0.471132    -1.381103    -0.697861      58.42
 H       0.238770    -2.208675    -1.104924      22.01
 C       2.297959     0.055513     0.316113      35.45
 C       3.775406     0.260526     0.218680     104.94
 H       3.950523    -0.100056    -0.784240      25.54
 O       4.146956     1.612763     0.379407     289.97
 H       4.995855     1.714276    -0.078927      27.82
 C       4.614114    -0.438928     1.260934      90.81
 H       4.381964     0.028147     2.169459      26.32
 O       4.181700    -1.944650     1.689412     155.53
 H       4.252910    -2.189369     2.754293      22.89
 C       6.089851    -0.564467     1.077291     107.70
 O       6.831040     0.697876     0.883767     137.74
 H       7.017641     1.306210     1.638835      19.72
 H       6.411931    -1.594259     0.415411      27.19
 H       6.320334    -0.840402     2.121885      30.23
55
name= lig-ACN-Water-frame_948
 C      -3.928311    -0.081594    -3.703584      69.95
 H      -3.613125    -1.044070    -4.163285      25.00
 C      -3.949155     1.328852    -1.732565      44.56
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 H      -3.949708     1.354049    -0.531707      18.65
 C      -4.039077     2.477375    -2.539001      24.82
 O      -3.863913     3.730097    -1.997313     288.71
 C      -3.717775     4.402120    -0.782385     129.08
 H      -4.215283     5.485674    -1.135651      21.90
 H      -2.719349     4.641636    -0.764088      24.80
 H      -4.505301     4.308839    -0.008289      22.86
 C      -3.910195     2.367168    -3.879335      -3.64
 O      -3.542376     3.487309    -4.590121     181.70
 H      -3.652827     4.364830    -4.035474      20.59
 C      -4.061193     1.079128    -4.573566      42.16
 H      -3.968310     1.110422    -5.628786      22.54
 C      -3.866269     0.030518    -2.301917      30.97
 C      -3.941575    -1.147104    -1.221193      67.97
 H      -4.539388    -1.992589    -1.675345      23.04
 O      -4.623005    -1.292373     0.281483     167.62
 H      -4.469954    -0.533032     0.728917      27.73
 C      -2.382759    -1.716147    -1.000743      55.79
 H      -1.998775    -1.590256    -2.070219      17.43
 C      -2.321845    -3.052940    -0.112995      93.47
 O      -3.310312    -4.161878    -0.764598     118.06
 H      -2.975137    -4.186087    -1.840487      25.72
 H      -2.800694    -3.032438     0.878749      22.08
 H      -1.342892    -3.659523    -0.320287      20.67
 C       1.716558    -1.161813    -0.329702     100.24
 H       2.462675    -2.078652    -0.536380      22.48
 C       1.431534     0.921401     0.876439      80.45
 H       1.728165     1.957886     1.304073      16.89
 C       0.120642     0.566427     0.868127       3.63
 O      -0.862487     1.375700     1.517716     247.94
 C      -0.596092     2.771971     1.618396      72.81
 H       0.155968     2.908691     0.927081      25.61
 H      -1.712404     3.290474     1.692942      19.59
 H       0.062748     2.562302     2.457302      21.05
 C      -0.544374    -0.516598     0.050402      10.40
 O      -1.825404    -0.681380    -0.077039     159.94
 C       0.383279    -1.324404    -0.556903      74.21
 H      -0.047591    -2.076346    -1.140303      20.26
 C       2.295983    -0.061124     0.193613      43.40
 C       3.795923     0.152586     0.150491      83.48
 H       4.256571    -0.130309    -0.760117      27.46
 O       4.207696     1.633296     0.356623     236.11
 H       5.137297     1.678524     0.044186      27.41
 C       4.591175    -0.490653     1.416054      90.14
 H       4.533511     0.253092     2.235629      26.71
 O       4.203305    -1.937319     1.641157     260.28
 H       4.133223    -1.979133     2.582735      28.85
 C       6.112109    -0.618575     1.123445      76.83
 O       6.887483     0.676975     0.886681     136.64
 H       6.932690     1.073049     1.767694      23.47
 H       6.412177    -1.230200     0.104492      27.10
 H       6.687944    -1.185241     2.012003      29.15
55
name= lig-ACN-Water-frame_949
 C      -3.956032    -0.130250    -3.648308      53.92
 H      -4.172637    -1.041093    -4.170961      22.69
 C      -3.976655     1.286967    -1.761840      78.58
 H      -3.907520     1.562713    -0.621739      20.51
 C      -3.975490     2.409452    -2.499251      -0.68
 O      -3.811058     3.809626    -2.122834     218.44
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 C      -3.694826     4.544839    -0.771386      98.97
 H      -4.175691     5.640037    -0.943626      23.12
 H      -2.709236     4.631167    -0.473748      29.24
 H      -3.884748     3.829673     0.020619      26.44
 C      -3.996058     2.318279    -3.966418      -8.35
 O      -3.549154     3.450932    -4.555519      70.64
 H      -3.824546     4.180504    -3.984699      16.55
 C      -3.994537     1.036970    -4.422505      74.06
 H      -4.115360     0.802092    -5.486213      26.42
 C      -3.968081    -0.032604    -2.178582      36.26
 C      -3.852574    -1.229385    -1.275809     107.46
 H      -4.376764    -2.030547    -1.936632      22.20
 O      -4.568852    -1.178589     0.089040     221.22
 H      -4.050067    -0.517548     0.629083      23.61
 C      -2.538180    -1.705764    -0.882322      83.70
 H      -1.794895    -1.960241    -1.706088      19.68
 C      -2.414653    -3.195547    -0.190524     109.43
 O      -3.201698    -4.230721    -0.795319     284.01
 H      -3.149001    -4.061251    -1.735906      32.39
 H      -2.486624    -2.923579     0.823074      25.64
 H      -1.278484    -3.420465    -0.157516      22.94
 C       1.774032    -1.224651    -0.416641      20.95
 H       2.584572    -2.003949    -1.007049      22.54
 C       1.416960     0.802887     0.768096      57.32
 H       1.791382     1.924318     1.072857      21.68
 C      -0.024479     0.494972     1.067045      23.68
 O      -0.942525     1.304564     1.581704     213.20
 C      -0.578068     2.752184     1.636017     101.93
 H      -0.365376     3.213624     0.745060      25.97
 H      -1.679493     3.337781     1.586402      23.04
 H      -0.324132     3.289253     2.507788      24.93
 C      -0.522215    -0.487135     0.234381      -7.42
 O      -2.044488    -0.595336    -0.104678     158.26
 C       0.315514    -1.416429    -0.451364      49.75
 H      -0.032188    -2.245061    -1.180744      19.86
 C       2.367332    -0.007243     0.184003      23.36
 C       3.953620     0.124162     0.224834      86.99
 H       4.314376    -0.363674    -0.631625      28.65
 O       4.203992     1.600025     0.271143     252.96
 H       5.193927     1.625935     0.405678      26.24
 C       4.594170    -0.571518     1.466031      99.33
 H       4.107600    -0.102452     2.391345      26.03
 O       4.200305    -1.865476     1.597621     286.53
 H       4.169298    -2.208665     2.465372      30.97
 C       6.237080    -0.620570     1.184924      94.43
 O       6.887728     0.585589     0.903458     138.48
 H       7.350424     1.216854     1.553762      21.62
 H       6.009096    -1.005084     0.064433      28.57
 H       6.820492    -1.567042     1.615577      28.75
55
name= lig-ACN-Water-frame_950
 C      -4.085005    -0.231383    -3.527342      38.35
 H      -4.230764    -1.214055    -3.872333      26.19
 C      -4.003173     1.343967    -1.521580      40.94
 H      -3.908830     1.432879    -0.450138      11.83
 C      -3.914296     2.512776    -2.441157     -12.67
 O      -3.780926     3.902142    -2.230193     225.20
 C      -3.592975     4.479346    -0.786139     134.74
 H      -4.213446     5.384880    -0.593050      25.19
 H      -2.579028     4.839603    -0.811297      26.75
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 H      -4.123027     3.847146    -0.163895      28.47
 C      -3.933433     2.298504    -3.846620     -22.88
 O      -3.603408     3.416850    -4.687392     150.40
 H      -3.880219     4.274653    -4.364686      21.18
 C      -3.976636     0.930173    -4.418943      51.24
 H      -3.840981     0.847342    -5.556178      19.79
 C      -4.034754    -0.078191    -2.173265       9.38
 C      -3.947174    -1.417151    -1.293688      99.07
 H      -4.432313    -2.416884    -1.663147      23.80
 O      -4.592650    -1.045723    -0.203113     225.09
 H      -3.986529    -0.495248     0.528946      17.61
 C      -2.486252    -1.810116    -0.849768      69.35
 H      -1.928819    -1.636153    -1.801806      22.11
 C      -2.449949    -3.167911    -0.183817     133.68
 O      -3.103595    -4.292378    -0.819824     250.18
 H      -3.287322    -4.146536    -1.720282      33.34
 H      -2.957961    -3.353501     0.672190      26.12
 H      -1.389504    -3.493669    -0.202436      25.70
 C       1.787008    -1.198095    -0.484273      71.51
 H       2.289569    -1.921556    -1.352526      22.95
 C       1.348367     0.749787     0.820360      52.79
 H       1.827197     1.577921     1.587711      20.44
 C      -0.021835     0.453700     0.986441     -18.49
 O      -1.007467     1.355162     1.724314     174.79
 C      -0.755652     2.846422     1.626080      90.27
 H      -0.136519     2.951342     0.803257      25.50
 H      -1.893207     3.142320     1.711924      20.61
 H      -0.085974     3.016629     2.418345      24.08
 C      -0.653907    -0.685794     0.240082     -12.30
 O      -1.996072    -0.505848    -0.002630     122.65
 C       0.433504    -1.457070    -0.343002      56.95
 H      -0.050557    -2.395534    -0.963507      19.85
 C       2.359288    -0.140045     0.158998      22.76
 C       3.926048     0.158303     0.296921      94.82
 H       4.377187    -0.275849    -0.547639      29.46
 O       4.234731     1.510754     0.169772     270.69
 H       4.995541     1.815769     0.683941      28.13
 C       4.700071    -0.503883     1.566244      80.31
 H       4.642557     0.150671     2.566705      25.35
 O       4.137580    -1.972149     1.526437     175.22
 H       4.450941    -2.282141     2.519941      25.08
 C       6.146225    -0.687237     1.131455      80.07
 O       6.969883     0.589824     0.906901     142.38
 H       7.127077     0.803004     1.899128      23.83
 H       6.245326    -1.289387     0.156717      27.23
 H       6.750307    -1.113283     2.111263      26.57
55
name= lig-ACN-Water-frame_951
 C      -4.199598    -0.195543    -3.545972      43.58
 H      -3.957611    -1.118517    -4.003315      20.96
 C      -3.993479     1.319867    -1.507916      66.78
 H      -4.029018     1.528431    -0.525684      21.69
 C      -3.873033     2.514694    -2.374060      -6.93
 O      -3.778251     3.957176    -2.180964     272.50
 C      -3.531432     4.363284    -0.886619     135.76
 H      -3.991164     5.300873    -0.945986      22.65
 H      -2.424275     4.400234    -0.728451      27.00
 H      -3.646202     3.740664    -0.073283      28.60
 C      -3.779510     2.219217    -3.812937      -6.44
 O      -3.700383     3.261768    -4.846974     183.11
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 H      -3.955671     4.091678    -4.354242      25.13
 C      -3.990030     0.937786    -4.334875      47.56
 H      -3.838701     0.856924    -5.487286      23.25
 C      -4.045314     0.009432    -2.096618      13.30
 C      -3.938439    -1.351841    -1.360374      90.03
 H      -4.481793    -2.094951    -2.064957      27.13
 O      -4.862586    -0.993906    -0.197562     123.87
 H      -4.246913    -0.244624     0.429964      19.48
 C      -2.468090    -1.760980    -0.954336      64.09
 H      -1.728297    -1.886015    -1.747760      22.74
 C      -2.395870    -3.178031    -0.061947      99.95
 O      -3.092323    -4.378408    -0.911791     173.15
 H      -2.686995    -4.169567    -1.880512      27.27
 H      -2.809551    -2.777206     0.754510      27.69
 H      -1.444968    -3.466524     0.285616      26.03
 C       1.744201    -1.191817    -0.530989       1.73
 H       2.574878    -1.903336    -1.037451      24.58
 C       1.354286     0.621182     1.015944      38.57
 H       1.679822     1.461039     1.773262      21.58
 C      -0.091237     0.530315     0.880791       2.25
 O      -0.962363     1.295832     1.756777     201.45
 C      -0.859344     2.792037     1.637605     119.74
 H      -0.617623     3.137113     0.658281      24.64
 H      -1.661024     3.570169     1.730914      24.57
 H      -0.358328     3.115281     2.474168      25.94
 C      -0.518417    -0.631841     0.291998      11.66
 O      -1.901232    -0.713584     0.044736     143.85
 C       0.343766    -1.559132    -0.348458      51.21
 H       0.090284    -2.578432    -0.939592      19.68
 C       2.293455    -0.098868     0.272292      16.05
 C       3.824105     0.067504     0.330452      96.23
 H       4.153550    -0.556399    -0.464883      29.45
 O       4.233941     1.551736     0.082143     184.90
 H       4.869940     1.661322     0.814381      27.04
 C       4.667306    -0.548861     1.457695      90.85
 H       4.629427    -0.092232     2.574725      24.02
 O       4.147176    -1.958351     1.545136     197.35
 H       4.336471    -2.459151     2.464590      24.97
 C       6.197251    -0.714934     1.171634      83.06
 O       6.976744     0.537022     0.919327     225.52
 H       7.195575     1.283289     1.604254      21.55
 H       6.441407    -1.452189     0.440520      26.59
 H       6.581026    -1.310987     2.205257      25.73
55
name= lig-ACN-Water-frame_952
 C      -4.135060    -0.078832    -3.502908      47.61
 H      -4.367947    -1.092732    -3.870301      22.85
 C      -3.956533     1.405568    -1.640202      76.11
 H      -4.050025     1.469653    -0.619775      20.37
 C      -3.798564     2.454158    -2.490169      21.92
 O      -3.838332     3.766207    -2.166570     311.56
 C      -3.354912     4.334746    -0.831754     149.89
 H      -3.701141     5.247494    -0.535492      25.94
 H      -2.230243     4.518792    -0.834455      26.17
 H      -3.915870     3.749659    -0.222143      30.06
 C      -3.720044     2.240646    -3.871485      17.84
 O      -3.800307     3.075334    -4.878666     186.89
 H      -3.794669     4.082823    -4.598627      25.87
 C      -4.002501     0.970790    -4.310574      58.91
 H      -4.167720     0.809434    -5.431010      24.01
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 C      -4.023799     0.092328    -2.159997      42.87
 C      -3.956888    -1.049864    -1.277666      83.31
 H      -4.294660    -1.992038    -1.839170      23.84
 O      -5.098301    -1.083448    -0.148721     145.38
 H      -4.697559    -0.538122     0.705799      22.79
 C      -2.422665    -1.815266    -0.898990      63.29
 H      -1.986514    -1.801518    -1.890182      21.87
 C      -2.487050    -3.168615    -0.104936     119.17
 O      -2.998787    -4.295153    -0.854260     184.05
 H      -2.523672    -4.441203    -1.895058      24.90
 H      -3.184525    -3.257026     0.596103      27.22
 H      -1.566655    -3.418290     0.226204      26.71
 C       1.714247    -1.181045    -0.390169      61.67
 H       2.453806    -1.893410    -0.862915      24.11
 C       1.340111     0.635597     1.246036      55.92
 H       1.813061     1.430234     1.839569      22.10
 C      -0.021363     0.593471     0.964323       1.45
 O      -0.936122     1.241440     1.677839     235.29
 C      -0.931527     2.760139     1.661577     101.81
 H      -0.528918     3.048092     0.669073      23.49
 H      -1.914503     2.540671     1.832460      20.31
 H      -0.276249     3.209130     2.293880      25.58
 C      -0.489147    -0.628517     0.143416     -13.95
 O      -1.867987    -0.985749     0.061184     169.69
 C       0.402908    -1.559343    -0.427702      58.35
 H      -0.173213    -2.414196    -0.802524      18.55
 C       2.182735    -0.120109     0.383976      30.08
 C       3.742063     0.043556     0.238575      70.33
 H       3.972642    -0.283288    -0.756084      26.07
 O       4.192800     1.474605     0.036636     219.90
 H       4.834630     1.813544     0.708982      28.51
 C       4.601479    -0.671388     1.418450      92.90
 H       4.107388     0.055922     2.268400      24.02
 O       4.170041    -1.949951     1.570693     296.08
 H       4.192179    -2.061611     2.487277      29.71
 C       6.291974    -0.687522     1.298513      89.23
 O       6.946303     0.492760     0.885466     214.57
 H       7.080331     0.950305     1.722347      25.84
 H       6.353293    -1.192369     0.416805      29.32
 H       6.908877    -1.280637     2.230887      26.73
55
name= lig-ACN-Water-frame_953
 C      -4.079269    -0.173369    -3.498421      45.16
 H      -4.644695    -1.126649    -3.785913      18.96
 C      -3.883293     1.457854    -1.643076      57.18
 H      -3.860577     1.767653    -0.572234      15.31
 C      -3.686341     2.487683    -2.601430      13.71
 O      -3.888444     3.797951    -2.121157     199.99
 C      -3.261659     4.232919    -0.783425     108.58
 H      -3.522312     5.136159    -0.983461      23.65
 H      -2.119022     3.945439    -0.828732      23.52
 H      -3.446267     3.831343     0.187206      28.20
 C      -3.759033     2.173011    -3.954695      10.04
 O      -3.859864     3.154685    -5.003177     170.33
 H      -3.889525     4.069319    -4.557241      24.08
 C      -4.033324     0.903188    -4.482323      31.83
 H      -4.307927     0.901278    -5.559433      20.35
 C      -3.964178     0.138284    -2.063553      16.70
 C      -4.071695    -1.123668    -1.061566      95.28
 H      -4.477878    -1.838245    -1.860281      23.55
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 O      -5.165026    -1.179575    -0.139844     237.87
 H      -4.870468    -0.870155     0.643224      31.90
 C      -2.616784    -1.769587    -0.798336      74.96
 H      -2.071131    -1.841576    -1.706124      23.27
 C      -2.635454    -3.143670    -0.165268     134.26
 O      -2.922694    -4.320200    -0.847556     306.42
 H      -2.562337    -4.184194    -1.817225      27.01
 H      -3.161547    -2.870409     0.659180      27.72
 H      -1.722700    -3.191953     0.239109      26.80
 C       1.778214    -1.252791    -0.250594      42.34
 H       2.489238    -1.723234    -0.861066      23.73
 C       1.405091     0.701294     1.299194      52.26
 H       1.648653     1.370596     2.034962      17.80
 C       0.026021     0.354780     1.012202       6.11
 O      -0.961626     1.202917     1.623182     244.07
 C      -1.056781     2.639115     1.659711      96.61
 H      -0.941252     3.155362     0.660309      23.61
 H      -1.881845     3.277531     1.950962      24.87
 H      -0.489230     2.873018     2.500640      24.44
 C      -0.542288    -0.585876     0.052385      23.55
 O      -1.780190    -1.029675     0.213268     178.15
 C       0.425067    -1.476045    -0.488124      72.77
 H       0.313509    -2.281674    -1.068989      22.99
 C       2.277731    -0.153103     0.498386      25.79
 C       3.755366     0.065527     0.127581      80.48
 H       3.995709    -0.601366    -0.733342      25.44
 O       4.109621     1.390260     0.008915     258.37
 H       4.674091     1.546150     0.776940      27.13
 C       4.602870    -0.553534     1.385063      76.87
 H       4.499430     0.057235     2.431591      23.31
 O       4.160887    -2.049313     1.626204     251.62
 H       4.029730    -2.353206     2.543491      27.45
 C       6.161837    -0.735337     1.254074      92.33
 O       6.935594     0.552302     0.910975     176.51
 H       7.274418     1.107878     1.599350      26.42
 H       6.421130    -1.520291     0.697793      33.15
 H       6.636816    -1.032300     2.386969      28.02
55
name= lig-ACN-Water-frame_954
 C      -4.116147    -0.202252    -3.440782      34.86
 H      -4.087780    -1.321285    -3.786662      23.17
 C      -3.717485     1.471002    -1.634362      33.06
 H      -3.733821     1.785162    -0.498473      18.20
 C      -3.689569     2.500279    -2.611113     -23.53
 O      -3.905586     3.881362    -2.052071     239.18
 C      -3.121091     4.154872    -0.884614     129.01
 H      -2.974994     5.131005    -0.630179      25.25
 H      -2.022397     3.866290    -1.062589      21.26
 H      -3.806353     3.804819    -0.090363      25.00
 C      -3.853444     2.200753    -4.163101     -30.61
 O      -3.889227     3.298471    -5.078141     178.55
 H      -4.227905     4.105708    -4.677880      23.63
 C      -4.049559     0.759197    -4.473342      52.79
 H      -4.177683     0.401830    -5.472406      27.88
 C      -3.954398     0.040372    -2.022481      19.62
 C      -4.167443    -1.239962    -1.149485      88.99
 H      -4.444334    -2.129965    -1.799360      26.16
 O      -5.167704    -1.263131    -0.060459     209.24
 H      -4.818111    -0.643249     0.583977      28.74
 C      -2.787664    -1.665327    -0.717120      77.93
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 H      -2.312094    -1.518119    -1.648610      20.78
 C      -2.670638    -3.045803     0.028043     102.82
 O      -2.919078    -4.413500    -0.939718     232.82
 H      -2.935141    -4.116611    -1.760599      32.59
 H      -3.378765    -3.270360     0.738814      26.54
 H      -1.756258    -3.225114     0.330102      27.24
 C       1.880939    -1.253882    -0.193362      41.59
 H       2.498207    -1.894744    -0.630196      24.32
 C       1.403651     0.575744     1.173780      67.54
 H       1.648810     1.365217     1.722576      24.55
 C      -0.017647     0.386115     1.057325       4.01
 O      -1.117809     1.075095     1.599720     200.84
 C      -1.053033     2.568244     1.695788      89.92
 H      -0.644932     2.958355     0.695694      23.84
 H      -2.145298     2.557520     1.977004      22.75
 H      -0.278692     3.034832     2.285465      23.54
 C      -0.415378    -0.635141     0.130359     -10.74
 O      -1.906443    -0.944092     0.389905      83.80
 C       0.493172    -1.443800    -0.587266      53.37
 H       0.083725    -2.090269    -1.266152      20.63
 C       2.383131    -0.188313     0.557638      40.89
 C       3.842476    -0.074270     0.303318      86.30
 H       4.103876    -0.551109    -0.717088      24.40
 O       4.076975     1.403584    -0.033630     223.53
 H       4.626142     1.860932     0.656380      26.90
 C       4.618566    -0.605773     1.377668      87.99
 H       4.252000     0.075620     2.300282      23.75
 O       4.163862    -2.025622     1.612774     205.77
 H       4.316896    -2.194507     2.678603      24.06
 C       6.100054    -0.684997     1.285066      94.36
 O       6.888370     0.560978     0.903160     214.76
 H       6.932029     1.043939     1.785113      25.44
 H       6.433566    -1.331037     0.599270      31.85
 H       6.276265    -1.018637     2.469200      28.42
55
name= lig-ACN-Water-frame_955
 C      -4.089573    -0.196020    -3.388158      53.01
 H      -3.946871    -1.285972    -3.740817      24.50
 C      -3.631171     1.328719    -1.741350      48.98
 H      -3.460313     1.527878    -0.567337      21.64
 C      -3.827812     2.497975    -2.681290     -24.82
 O      -3.871950     3.865495    -2.177711     228.44
 C      -2.972163     4.123796    -0.933672      79.20
 H      -2.820969     5.116626    -0.922559      24.25
 H      -2.169873     3.311019    -0.972790      22.04
 H      -3.459696     3.695835     0.000209      23.79
 C      -3.983461     2.262517    -4.101728      -9.86
 O      -3.924491     3.291511    -5.100271     221.96
 H      -4.164399     4.164492    -4.728377      22.48
 C      -4.035735     0.821579    -4.388978      50.81
 H      -3.847309     0.447660    -5.338964      24.21
 C      -4.051010     0.060475    -2.056658      31.50
 C      -4.201605    -1.240174    -1.167370      75.00
 H      -4.565100    -2.038400    -1.825873      23.84
 O      -5.143510    -1.287352     0.006306     160.31
 H      -4.765853    -0.504441     0.722069      21.84
 C      -2.698036    -1.720544    -0.530298      71.81
 H      -1.978551    -1.892597    -1.315878      19.74
 C      -2.718472    -3.209301     0.018553     107.51
 O      -2.917251    -4.337321    -0.934420     293.01
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 H      -3.023794    -4.026607    -1.843688      30.16
 H      -3.456456    -3.139519     0.817594      25.14
 H      -1.810232    -3.229280     0.491610      27.97
 C       1.882786    -1.383625    -0.352422      41.91
 H       2.540973    -2.049965    -0.618559      23.70
 C       1.354629     0.633903     1.145679      54.44
 H       1.816218     1.480157     1.482475      21.77
 C      -0.045075     0.387002     0.986273       8.17
 O      -1.120364     0.967096     1.627992     224.22
 C      -1.030872     2.434546     1.698872     108.65
 H      -0.979732     2.851245     0.645034      22.24
 H      -2.061478     2.921980     1.970750      22.39
 H      -0.508242     2.704422     2.673603      22.25
 C      -0.515747    -0.765925     0.321797      -0.13
 O      -1.997494    -0.794183     0.407975     124.70
 C       0.482867    -1.406718    -0.547161      69.49
 H       0.247240    -2.260026    -1.210468      21.00
 C       2.306564    -0.340278     0.501121       3.41
 C       3.871041     0.020808     0.329115      71.33
 H       4.243649    -0.607474    -0.639757      24.08
 O       4.099166     1.383960    -0.048482     250.89
 H       4.546130     1.958087     0.622235      26.37
 C       4.619430    -0.660456     1.570308      99.10
 H       4.312292    -0.076989     2.562558      25.03
 O       4.191733    -1.955276     1.590758     238.91
 H       4.396497    -2.407784     2.564102      25.08
 C       6.201618    -0.632758     1.357778     101.49
 O       6.768046     0.539645     0.970540     216.29
 H       6.952546     1.322243     1.632587      21.98
 H       6.187608    -1.258330     0.539085      31.67
 H       7.003685    -1.165920     2.103892      29.61
55
name= lig-ACN-Water-frame_956
 C      -4.076039    -0.183758    -3.542638      51.70
 H      -4.323907    -1.171796    -4.018460      22.59
 C      -3.721316     1.395643    -1.784281      48.74
 H      -3.231795     1.730479    -0.770921      23.64
 C      -3.938993     2.473204    -2.586797      19.99
 O      -3.759215     3.765398    -2.306283     216.91
 C      -2.891470     3.980815    -1.038599     125.30
 H      -2.600793     4.949646    -1.252066      26.60
 H      -1.873959     3.637030    -1.248558      24.98
 H      -3.425584     4.113393    -0.029832      25.63
 C      -4.090706     2.253135    -3.984743       8.90
 O      -3.985096     3.148518    -5.052860     183.36
 H      -3.979038     4.138059    -4.752518      22.16
 C      -3.991300     0.957460    -4.384510      63.68
 H      -3.858821     0.954769    -5.426253      21.38
 C      -4.098001     0.012672    -2.030311       7.83
 C      -4.040021    -1.208738    -0.987074      95.35
 H      -4.428938    -1.979523    -1.627703      23.43
 O      -5.086942    -1.228259     0.014076     168.74
 H      -4.623344    -0.748848     0.962025      21.74
 C      -2.581429    -1.879153    -0.541852      58.87
 H      -2.004953    -1.855659    -1.501966      19.33
 C      -2.745425    -3.287382     0.106451     122.48
 O      -2.942987    -4.220432    -0.916034     220.28
 H      -2.640054    -3.757507    -1.893240      23.44
 H      -3.661614    -3.430227     0.727587      25.65
 H      -1.919240    -3.713559     0.620054      25.60
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 C       1.750717    -1.407409    -0.400222      41.13
 H       2.251572    -1.946001    -1.104293      21.25
 C       1.389108     0.594731     1.002077      51.65
 H       1.554996     1.493986     1.622528      16.92
 C      -0.037508     0.288190     1.001301       5.63
 O      -1.084609     0.966922     1.698095     240.22
 C      -1.074119     2.375759     1.761536     116.52
 H      -0.416304     2.778052     0.945796      23.12
 H      -2.069889     2.781605     2.051714      23.37
 H      -0.135842     2.631456     2.407360      21.02
 C      -0.606239    -0.843037     0.361995       6.05
 O      -2.007068    -0.773282     0.284636     146.39
 C       0.292488    -1.614203    -0.437968      66.19
 H      -0.225178    -2.431545    -1.119463      17.76
 C       2.283440    -0.275950     0.391640      30.42
 C       3.791355     0.031076     0.385390      59.84
 H       4.302945    -0.742551    -0.417588      22.24
 O       4.132274     1.397447    -0.032728     238.01
 H       4.435910     1.709578     0.831845      24.23
 C       4.742491    -0.520650     1.814379      77.76
 H       4.519431    -0.176391     2.880718      23.63
 O       4.202964    -2.009579     1.583177     269.46
 H       4.139030    -2.513336     2.403014      28.08
 C       6.219786    -0.744351     1.383461      85.07
 O       6.729078     0.687065     0.997298     168.38
 H       6.969090     1.043270     1.930995      24.36
 H       6.381105    -1.272882     0.471553      31.26
 H       6.711147    -1.294936     2.310440      29.40
55
name= lig-ACN-Water-frame_957
 C      -4.151406    -0.161857    -3.533105      56.10
 H      -4.226052    -1.149347    -3.967990      23.72
 C      -3.892419     1.354530    -1.606797      46.05
 H      -3.558168     1.503632    -0.552775      15.41
 C      -4.028996     2.431078    -2.589472       7.07
 O      -3.596409     3.767012    -2.285889     250.56
 C      -2.763207     4.055755    -1.259993     105.13
 H      -2.456912     5.084065    -1.240149      24.42
 H      -2.161232     3.192698    -1.028547      25.35
 H      -3.526657     3.717879    -0.406563      22.59
 C      -4.125057     2.201506    -3.948873       7.35
 O      -4.060039     3.082892    -4.979084     183.72
 H      -4.177368     4.092358    -4.729509      22.80
 C      -4.018259     0.888958    -4.465013      56.64
 H      -4.090197     0.615591    -5.517417      18.36
 C      -3.944860     0.007898    -2.158977       0.16
 C      -3.933824    -1.294990    -1.021313      93.22
 H      -4.279559    -2.140314    -1.574173      27.04
 O      -4.976930    -1.141764     0.065037     154.02
 H      -4.552844    -0.377591     0.888678      16.22
 C      -2.621179    -1.828979    -0.587386      72.98
 H      -2.144223    -2.144696    -1.583318      21.40
 C      -2.730183    -3.265357     0.220214     108.51
 O      -3.018467    -4.205968    -1.005862     104.90
 H      -2.328765    -3.876312    -1.875429      23.36
 H      -3.698432    -3.099765     0.869959      24.87
 H      -1.803603    -3.417240     0.847668      24.16
 C       1.523783    -1.335506    -0.371463      37.28
 H       2.284323    -1.991096    -0.863551      24.22
 C       1.250023     0.535658     0.948959      49.08
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 H       1.836353     1.359820     1.536692      18.75
 C      -0.062930     0.211220     1.083191      25.35
 O      -1.021601     0.902299     1.755872     205.64
 C      -0.888775     2.453469     1.840794      99.85
 H      -0.933811     2.854614     0.846460      24.59
 H      -1.922059     2.612555     1.964442      25.66
 H      -0.636686     2.964867     2.849938      21.05
 C      -0.613355    -0.842968     0.278314      11.95
 O      -1.945468    -0.897362     0.155173     180.92
 C       0.169947    -1.831578    -0.287338      75.82
 H      -0.162479    -2.731855    -1.078100      17.65
 C       2.243466    -0.258337     0.214455      22.53
 C       3.818654    -0.036887     0.534315      61.83
 H       4.363207    -0.678178    -0.381111      20.99
 O       4.133227     1.389684     0.046937     222.85
 H       4.489287     2.041047     0.698528      23.68
 C       4.681262    -0.647993     1.710863     104.49
 H       4.624345    -0.093587     2.654702      23.60
 O       4.233285    -1.993297     1.635126     331.87
 H       4.124956    -2.359728     2.495516      29.35
 C       6.179230    -0.634109     1.411304      88.80
 O       6.741520     0.713639     1.115055     297.22
 H       6.955774     1.270799     1.959262      22.86
 H       6.242724    -1.393710     0.542557      29.24
 H       6.868276    -0.992191     2.217783      28.28
55
name= lig-ACN-Water-frame_958
 C      -4.125588    -0.281500    -3.469009      42.02
 H      -4.033170    -1.284520    -3.752833      24.25
 C      -4.035755     1.266701    -1.569489      59.95
 H      -4.180958     1.442268    -0.550481      22.35
 C      -3.962944     2.393221    -2.498237     -32.58
 O      -3.560750     3.801253    -2.456196     172.41
 C      -2.685459     3.997953    -1.184027     108.77
 H      -2.126100     4.946208    -1.478445      24.84
 H      -1.776599     3.508714    -1.313416      26.45
 H      -3.047437     4.281314    -0.109278      24.62
 C      -4.089727     2.066774    -4.009877     -39.55
 O      -4.147013     3.155308    -4.946123     163.87
 H      -4.237725     4.027649    -4.510169      21.82
 C      -4.205204     0.729530    -4.462965      61.64
 H      -4.161652     0.571688    -5.593724      21.94
 C      -3.857234    -0.028869    -2.063494      28.09
 C      -4.059616    -1.297781    -1.220288      87.17
 H      -4.628264    -2.024751    -1.787410      26.58
 O      -4.832375    -1.086057     0.009347     154.35
 H      -4.386516    -0.268654     0.730994      17.19
 C      -2.648528    -1.910199    -0.650092      88.49
 H      -1.851764    -2.020436    -1.486005      22.55
 C      -2.781537    -3.162553     0.010103     123.39
 O      -3.088656    -4.203862    -0.913561     231.39
 H      -2.435744    -4.070327    -1.641888      30.60
 H      -3.559634    -3.276673     0.934061      24.68
 H      -1.725192    -3.545104     0.403268      23.23
 C       1.610660    -1.484265    -0.412804      48.44
 H       2.266377    -2.405424    -0.682444      23.73
 C       1.287839     0.532682     1.000414      57.78
 H       1.459364     1.561150     1.578730      19.98
 C      -0.106281     0.167100     1.041477      -7.26
 O      -0.958537     0.974420     1.887556     209.03
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 C      -0.968994     2.444361     1.877705     119.34
 H      -0.306300     2.842822     1.126534      26.09
 H      -1.885843     2.790432     2.047299      27.27
 H      -0.107983     2.612359     2.564186      22.74
 C      -0.611158    -0.914775     0.242783      16.64
 O      -1.984181    -0.882592     0.149693     177.81
 C       0.288604    -1.846237    -0.223013      68.57
 H      -0.074420    -2.984629    -0.625110      19.61
 C       2.055914    -0.277083     0.239434       5.69
 C       3.828345    -0.009416     0.369264      72.59
 H       4.184315    -0.640562    -0.626487      24.18
 O       4.094139     1.339638     0.155668     233.81
 H       4.473913     1.670258     1.005040      24.44
 C       4.531591    -0.657480     1.618904      97.24
 H       4.098006    -0.226235     2.503476      24.87
 O       4.252968    -2.054241     1.724612     265.24
 H       4.319606    -2.451188     2.739680      24.77
 C       6.185460    -0.501737     1.419368      86.13
 O       6.747028     0.728057     1.184622     275.47
 H       6.884573     1.205973     2.060333      23.74
 H       6.553864    -0.995877     0.404356      26.68
 H       6.555053    -1.069546     2.281448      29.98
55
name= lig-ACN-Water-frame_959
 C      -3.979801    -0.411405    -3.440733      51.58
 H      -4.024984    -1.414069    -3.770382      22.46
 C      -4.087997     1.360918    -1.632887      70.02
 H      -4.295327     1.624637    -0.676176      21.54
 C      -3.848709     2.313917    -2.677923       6.20
 O      -3.571417     3.700760    -2.409448     194.58
 C      -2.515257     4.061381    -1.257936      72.87
 H      -2.285033     5.166847    -1.631485      22.02
 H      -1.984737     3.166655    -1.096066      24.61
 H      -3.248873     4.058809    -0.281039      22.33
 C      -4.082292     2.043007    -3.985005       2.98
 O      -4.227799     3.099920    -4.864242     218.29
 H      -4.045486     3.948344    -4.475846      21.65
 C      -4.343773     0.660084    -4.355237      33.66
 H      -4.497810     0.360257    -5.475877      28.32
 C      -4.018858    -0.064216    -2.083907      30.00
 C      -4.054562    -1.272024    -1.220857     105.11
 H      -4.562958    -2.069639    -1.820969      24.08
 O      -4.816035    -1.110543    -0.138069     234.08
 H      -4.378194    -0.548532     0.637517      22.61
 C      -2.659443    -1.836281    -0.912038      55.20
 H      -2.060158    -1.964359    -1.898006      20.50
 C      -2.737988    -3.237551    -0.070410      94.88
 O      -3.235132    -4.303516    -0.854870     268.50
 H      -2.893653    -4.292457    -1.660420      35.03
 H      -3.579595    -3.052276     0.866266      23.05
 H      -1.694584    -3.287903     0.520916      23.38
 C       1.801509    -1.617027    -0.275856      28.19
 H       2.706143    -2.189663    -0.851482      20.54
 C       1.212137     0.494747     1.025894      41.82
 H       1.769073     1.385578     1.510578      19.17
 C      -0.153870     0.303290     1.029447      11.48
 O      -0.991446     0.951306     1.944870     238.37
 C      -0.840999     2.396746     1.877902     131.39
 H      -0.727389     2.688702     0.856911      26.25
 H      -1.777400     2.801805     1.995482      26.54
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 H      -0.495689     2.899632     2.716836      25.28
 C      -0.633207    -0.883141     0.358115     -12.56
 O      -2.121740    -0.857709     0.197585      91.66
 C       0.365093    -1.867816    -0.263957      69.77
 H      -0.079486    -2.999954    -0.426544      19.57
 C       2.244963    -0.381845     0.276526      21.44
 C       3.592573    -0.123414     0.104344      72.53
 H       4.168687    -0.564249    -0.864394      24.34
 O       4.064364     1.337619     0.284432     141.74
 H       4.382693     1.463514     1.186571      26.08
 C       4.458546    -0.610720     1.531164      70.38
 H       4.194688     0.036878     2.311812      26.33
 O       4.262187    -2.123918     1.719456     201.81
 H       4.455822    -2.363459     2.787809      24.15
 C       6.035087    -0.552858     1.433950      85.40
 O       6.769041     0.867043     1.249411     198.84
 H       6.832115     1.234022     2.235442      20.47
 H       6.251308    -1.359388     0.535782      27.74
 H       6.503298    -0.978902     2.271318      31.96
55
name= lig-ACN-Water-frame_960
 C      -3.979388    -0.349585    -3.484574      52.80
 H      -3.903289    -1.399726    -3.822065      25.52
 C      -4.049488     1.319180    -1.779027      66.58
 H      -3.960770     1.615036    -0.783847      16.35
 C      -3.728355     2.316017    -2.659796      29.38
 O      -3.556311     3.583455    -2.296944     280.80
 C      -2.589480     4.029600    -1.404395      98.70
 H      -1.831093     4.970297    -1.613163      21.15
 H      -1.670570     3.434421    -1.291123      23.51
 H      -3.148938     4.317769    -0.305578      23.55
 C      -4.139180     1.944532    -4.033497       3.59
 O      -4.299745     2.979235    -4.881018     182.62
 H      -4.145247     3.807340    -4.291269      23.16
 C      -4.332508     0.642441    -4.350945      63.82
 H      -4.863124     0.435566    -5.354148      23.19
 C      -4.156516     0.005388    -2.159015      41.65
 C      -4.018309    -1.304267    -1.281210      81.53
 H      -4.391502    -2.200398    -1.890059      22.51
 O      -4.976694    -1.167511    -0.086808     192.89
 H      -4.643667    -0.486858     0.429009      29.51
 C      -2.601314    -1.782942    -0.915152      66.43
 H      -1.858058    -1.568663    -1.756171      17.66
 C      -2.711131    -3.167354    -0.151873      80.84
 O      -3.402415    -4.482584    -0.815987     171.40
 H      -3.109595    -4.256812    -1.840783      26.17
 H      -3.545687    -2.779256     0.696394      21.60
 H      -1.683910    -3.678338     0.252803      22.44
 C       1.729246    -1.669396    -0.117587      29.21
 H       2.343271    -2.468667    -0.789808      17.31
 C       1.359338     0.411957     0.953454      87.09
 H       1.730397     1.292230     1.452483      18.24
 C      -0.115090     0.239147     1.057818      37.87
 O      -1.019496     0.920312     1.939060     245.83
 C      -0.898969     2.447555     1.834188     103.93
 H      -0.494393     2.692957     0.898720      24.63
 H      -1.867630     2.583984     2.010278      22.30
 H      -0.076423     2.798724     2.436645      21.13
 C      -0.668801    -0.873892     0.353496      28.89
 O      -2.072763    -0.935166     0.164284     207.89
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 C       0.355193    -1.799636    -0.191757     100.19
 H       0.031327    -2.636826    -0.957987      16.67
 C       2.156687    -0.433383     0.348660      26.80
 C       3.747426    -0.074648     0.226993      79.01
 H       3.991995    -0.424376    -0.880780      21.63
 O       3.962393     1.319812     0.289190     219.87
 H       4.261180     1.498733     1.217938      26.25
 C       4.432068    -0.724718     1.356972     105.33
 H       3.897816    -0.245002     2.108748      25.87
 O       4.258220    -2.034625     1.654229     326.93
 H       4.234387    -2.410115     2.552287      28.46
 C       5.949717    -0.500308     1.432019      90.16
 O       6.686660     0.826867     1.306506     221.49
 H       6.792498     1.310354     2.203190      22.78
 H       6.527645    -1.063002     0.470957      28.11
 H       6.196655    -0.883880     2.323930      32.74
55
name= lig-ACN-Water-frame_961
 C      -4.152367    -0.364205    -3.585312      38.29
 H      -3.978622    -1.467783    -3.910048      23.16
 C      -3.920203     1.210822    -1.681596      51.93
 H      -3.830595     1.387174    -0.584814      10.36
 C      -3.735596     2.206976    -2.683011      20.00
 O      -3.610880     3.594869    -2.341028     189.52
 C      -2.521179     4.035050    -1.391318      74.88
 H      -2.548996     4.962423    -2.101224      19.76
 H      -1.791155     3.148749    -1.356385      21.08
 H      -2.876755     4.357989    -0.214827      22.47
 C      -4.107808     1.974188    -4.005480       1.37
 O      -4.366444     2.937617    -4.986873     191.14
 H      -4.555082     3.889945    -4.678625      26.62
 C      -4.308778     0.666291    -4.567092      40.46
 H      -4.555867     0.515406    -5.655959      18.88
 C      -4.097439    -0.143530    -2.150959      25.84
 C      -4.148171    -1.252071    -1.253196      85.98
 H      -4.632310    -2.139520    -1.816739      27.08
 O      -5.086099    -1.252081    -0.073562     142.02
 H      -4.855301    -0.502683     0.491133      28.02
 C      -2.507673    -1.802169    -0.812798      63.70
 H      -1.977825    -1.927449    -1.779710      20.22
 C      -2.785928    -3.243753    -0.286408      91.76
 O      -3.493311    -4.470634    -0.770958     160.23
 H      -3.396538    -4.624894    -1.912716      27.09
 H      -3.216005    -3.217742     0.855698      24.22
 H      -1.615888    -3.599698    -0.042553      21.70
 C       1.574862    -1.694346    -0.056901      29.14
 H       2.220234    -2.625632    -0.371021      21.11
 C       1.281489     0.491239     1.031840     111.84
 H       1.587814     1.390253     1.357560      17.55
 C      -0.042111     0.091757     1.138819      -4.95
 O      -0.978006     0.923473     1.850378     259.56
 C      -0.928456     2.424231     1.769432      95.95
 H      -0.763111     2.765407     0.810654      24.23
 H      -1.683170     3.076430     2.069409      23.87
 H      -0.288492     2.711016     2.619767      20.39
 C      -0.620544    -0.871151     0.295747      22.10
 O      -1.941331    -0.972806     0.176444     247.62
 C       0.168020    -1.818436    -0.223482      68.48
 H      -0.249816    -2.464006    -0.976698      18.46
 C       2.267550    -0.508842     0.381941      55.02
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 C       3.713906    -0.079553     0.246954      76.84
 H       4.280644    -0.423859    -0.716439      21.50
 O       3.873889     1.362358     0.262527     246.19
 H       4.033589     1.794485     1.129946      26.99
 C       4.474530    -0.634817     1.431674     117.92
 H       4.202509    -0.136767     2.310284      26.47
 O       4.205213    -2.132019     1.500236     314.68
 H       4.088745    -2.139502     2.413148      29.73
 C       6.029665    -0.471153     1.466562      99.16
 O       6.560559     0.781740     1.370881     305.95
 H       6.523687     1.186268     2.299679      26.89
 H       6.501293    -1.242810     0.584897      29.69
 H       6.369819    -0.947356     2.283926      33.61
55
name= lig-ACN-Water-frame_962
 C      -4.350490    -0.413950    -3.697599      41.66
 H      -4.566277    -1.513234    -4.089121      24.08
 C      -3.749734     1.074476    -1.667400      52.74
 H      -3.704948     1.346309    -0.531410      21.00
 C      -3.854759     2.199551    -2.637425     -24.56
 O      -3.729993     3.553203    -2.394113     169.31
 C      -2.500685     4.099317    -1.469108      59.73
 H      -1.775742     4.998859    -1.452870      21.31
 H      -1.608314     3.315007    -1.505875      22.34
 H      -3.135339     3.973599    -0.385365      21.58
 C      -4.116736     1.992691    -4.112795     -15.57
 O      -4.385597     2.963757    -5.113399     199.64
 H      -4.535358     3.818859    -4.731589      26.25
 C      -4.197386     0.661912    -4.583985      49.72
 H      -4.014584     0.532683    -5.627281      20.53
 C      -4.045023    -0.153135    -2.236827      -5.13
 C      -4.153490    -1.419416    -1.110341      86.64
 H      -4.480069    -2.309205    -1.776683      24.85
 O      -5.131882    -1.276416    -0.085920     213.48
 H      -4.666453    -0.678013     0.718469      23.09
 C      -2.792381    -1.914471    -0.846526      47.36
 H      -2.141642    -1.732614    -1.691586      23.05
 C      -2.696765    -3.446803    -0.209503     101.86
 O      -3.605553    -4.361655    -0.783522     238.24
 H      -3.246843    -4.550373    -1.678161      31.82
 H      -3.086827    -3.220907     0.900046      24.45
 H      -1.572740    -3.929159    -0.282213      21.93
 C       1.584989    -1.714739    -0.080442      35.75
 H       2.343888    -2.490066    -0.326588      19.24
 C       1.330902     0.423574     1.056703      83.42
 H       1.670288     1.300599     1.445106      21.15
 C      -0.054617     0.182885     1.198182       6.30
 O      -1.037475     0.955098     1.759501     237.19
 C      -0.878970     2.404912     1.741998      99.43
 H      -0.653430     2.669620     0.752465      26.39
 H      -1.877825     2.286487     2.023845      21.81
 H      -0.000534     2.892255     2.283182      22.49
 C      -0.582595    -0.898904     0.327045      11.01
 O      -2.006923    -0.951981     0.214234     139.23
 C       0.211768    -1.915313    -0.350017      74.25
 H      -0.094524    -2.837386    -0.564833      19.34
 C       2.120591    -0.478008     0.455522      36.64
 C       3.662596    -0.096502     0.296589      61.49
 H       4.037477    -0.546634    -0.652815      22.27
 O       3.792910     1.451033     0.185016     231.34
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 H       3.622218     1.614819     1.125020      26.58
 C       4.570116    -0.614387     1.604119      92.43
 H       4.131566    -0.246046     2.474016      27.36
 O       4.160171    -2.140025     1.409495     258.39
 H       4.036468    -2.900309     2.149232      27.90
 C       6.087501    -0.700665     1.514968      90.09
 O       6.489121     0.878074     1.440573     125.13
 H       6.572246     1.244099     2.406896      24.08
 H       6.389201    -1.137655     0.394973      29.09
 H       6.517056    -1.113588     2.319065      33.01
55
name= lig-ACN-Water-frame_963
 C      -4.418175    -0.417203    -3.586043      38.24
 H      -4.855111    -1.393327    -4.039101      26.72
 C      -3.673094     1.104679    -1.934149      36.92
 H      -3.253731     1.146450    -0.826859      19.56
 C      -3.940649     2.222804    -2.718089       6.37
 O      -3.746559     3.645478    -2.387300     187.05
 C      -2.610680     3.969132    -1.505129      82.96
 H      -2.640961     5.012387    -1.927530      21.92
 H      -1.741084     3.109543    -1.600224      22.98
 H      -2.938683     4.018660    -0.232629      22.75
 C      -4.129201     1.950932    -4.126657      -8.94
 O      -4.318346     2.981235    -5.150599     182.25
 H      -4.042866     3.866478    -4.757068      23.75
 C      -4.098948     0.634512    -4.561989      70.85
 H      -4.199872     0.423177    -5.567778      16.85
 C      -4.110467    -0.348358    -2.257475       5.38
 C      -4.216295    -1.518055    -1.245174      81.74
 H      -4.754672    -2.388997    -1.727758      24.66
 O      -5.122477    -1.262018    -0.051018     149.47
 H      -4.540782    -0.835499     0.770159      23.80
 C      -2.772258    -2.059980    -0.699587      81.62
 H      -2.305476    -2.065885    -1.665396      24.56
 C      -2.635224    -3.463672    -0.095728     109.73
 O      -3.727140    -4.281848    -0.826485     231.29
 H      -3.378132    -4.443688    -1.624459      36.38
 H      -2.732381    -3.563099     1.050304      26.79
 H      -1.556311    -3.974250    -0.325608      24.33
 C       1.737174    -1.680418    -0.176408      19.13
 H       2.376039    -2.371641    -0.629368      20.85
 C       1.259076     0.422996     1.172517      67.99
 H       1.744180     1.222678     1.778564      16.31
 C      -0.151862     0.126134     0.998584      20.29
 O      -1.060575     0.938018     1.715177     217.94
 C      -0.914842     2.405529     1.674303     108.65
 H      -0.771221     2.814086     0.681931      25.75
 H      -1.554620     3.255633     2.036426      24.78
 H      -0.134634     2.572414     2.501791      23.03
 C      -0.680419    -1.019358     0.326095       8.25
 O      -2.149914    -0.965652     0.234051     141.61
 C       0.321715    -1.910677    -0.241625      76.23
 H       0.008886    -2.742367    -0.656174      19.56
 C       2.149024    -0.514927     0.463348      38.43
 C       3.643991    -0.037523     0.467262      81.60
 H       4.050596    -0.433072    -0.436511      25.73
 O       3.725619     1.372049     0.147440     213.35
 H       3.507921     2.100800     0.782789      25.39
 C       4.479332    -0.851629     1.637538      99.46
 H       4.243434    -0.486280     2.624400      27.04
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 O       4.129408    -2.113125     1.335447     250.68
 H       4.431728    -2.535169     2.297569      25.16
 C       6.099256    -0.637931     1.544157      88.27
 O       6.445247     0.838265     1.515279     203.11
 H       6.616440     1.150498     2.485627      22.89
 H       6.539146    -1.004901     0.483650      31.04
 H       6.581331    -1.313841     2.184458      33.23
55
name= lig-ACN-Water-frame_964
 C      -4.415175    -0.480075    -3.594953      39.13
 H      -4.726960    -1.488256    -3.968362      26.62
 C      -3.683714     1.019031    -2.039235      47.26
 H      -3.061061     1.385552    -1.142834      22.72
 C      -3.925373     2.238782    -2.858433       6.59
 O      -3.817543     3.560293    -2.405974     264.42
 C      -2.783560     3.895981    -1.546665     105.65
 H      -2.215144     4.920110    -1.711756      23.39
 H      -1.729215     3.345937    -1.825171      23.21
 H      -3.025010     4.027892    -0.280954      22.95
 C      -4.102247     1.995862    -4.197857      10.05
 O      -4.194179     2.943466    -5.095764     208.89
 H      -3.807535     3.888499    -4.886815      22.43
 C      -4.202798     0.546061    -4.525143      59.64
 H      -4.453094     0.365110    -5.511964      16.29
 C      -4.123591    -0.271246    -2.212096      22.76
 C      -4.298320    -1.534920    -1.225019      72.00
 H      -4.758366    -2.333673    -1.833466      23.64
 O      -5.070625    -1.248034    -0.057611     234.17
 H      -4.545930    -0.640200     0.439249      28.25
 C      -2.641957    -2.088297    -0.624135      67.17
 H      -1.860046    -2.090304    -1.333498      22.52
 C      -2.735106    -3.536219    -0.063022     114.87
 O      -3.765381    -4.209944    -0.774820     190.08
 H      -3.470616    -4.321858    -1.834170      28.87
 H      -2.957441    -3.684081     0.996576      27.39
 H      -1.677389    -3.997913    -0.368329      24.43
 C       1.759430    -1.556906    -0.244715      32.67
 H       2.424206    -2.076397    -0.850268      23.01
 C       1.142690     0.232333     1.141180      41.12
 H       1.196268     1.057781     1.970277      14.86
 C      -0.235573     0.157014     0.920132      14.55
 O      -1.175487     0.930730     1.649243     205.85
 C      -0.838816     2.446511     1.641454      89.34
 H      -0.397437     2.587902     0.622350      23.82
 H      -1.941159     2.684896     1.954351      21.69
 H       0.119788     2.677135     2.247332      22.63
 C      -0.753886    -1.034022     0.313084       8.50
 O      -2.169405    -1.105376     0.188396     190.05
 C       0.290117    -1.941717    -0.137297      89.29
 H       0.104972    -2.516431    -0.954281      20.46
 C       2.243767    -0.434090     0.560308      33.93
 C       3.652077    -0.054134     0.581155     101.60
 H       4.117160    -0.536773    -0.236274      26.82
 O       3.728758     1.319077     0.128774     223.20
 H       3.473468     1.847818     0.939222      25.83
 C       4.488278    -0.753507     1.626140      97.35
 H       4.124745    -0.707433     2.645306      25.40
 O       4.123919    -2.257037     1.348100     237.25
 H       4.304399    -2.851892     2.035465      30.65
 C       6.005109    -0.534604     1.490120      99.03
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 O       6.442479     0.754233     1.620947     304.19
 H       6.352866     1.093196     2.587757      24.07
 H       6.286382    -0.962219     0.430286      28.96
 H       6.509581    -0.940920     2.314413      29.71
55
name= lig-ACN-Water-frame_965
 C      -4.392668    -0.539508    -3.632826      35.44
 H      -4.472528    -1.560864    -3.962955      22.42
 C      -3.691787     1.127516    -1.876764      45.35
 H      -3.496421     1.240582    -0.801704      21.50
 C      -3.809338     2.092147    -2.834877       1.12
 O      -3.946307     3.447831    -2.484227     184.53
 C      -2.740010     3.913669    -1.531186      80.78
 H      -2.630782     5.020630    -1.623078      23.48
 H      -2.025112     2.978378    -1.480577      21.79
 H      -3.412496     3.511337    -0.521085      21.47
 C      -4.072132     1.832231    -4.256335     -13.67
 O      -4.075433     2.953372    -5.194318     175.35
 H      -4.047108     3.739656    -4.599725      18.70
 C      -4.446837     0.550590    -4.595669      53.44
 H      -4.416144     0.319597    -5.651444      30.44
 C      -4.115874    -0.243652    -2.251191       4.34
 C      -4.087461    -1.438925    -1.166367      95.30
 H      -4.611242    -2.247599    -1.645733      24.67
 O      -5.016186    -1.211348    -0.069424     204.69
 H      -4.777229    -0.456512     0.410584      30.35
 C      -2.692495    -2.126353    -0.795122      75.25
 H      -2.365123    -2.131854    -1.790226      19.46
 C      -2.799761    -3.587476    -0.044306     107.48
 O      -3.851816    -4.245252    -0.759464     182.40
 H      -3.463161    -4.104804    -1.838072      27.38
 H      -3.195885    -3.304845     0.930226      25.02
 H      -1.922014    -4.301015     0.116012      25.06
 C       1.582066    -1.439169    -0.202828      50.10
 H       2.235816    -2.014556    -0.813940      23.42
 C       1.059255     0.232925     1.223788      96.30
 H       1.566804     1.069666     1.920925      18.00
 C      -0.328426     0.081566     0.992845      26.62
 O      -1.168723     0.955389     1.538313     238.42
 C      -0.787207     2.355627     1.581186      99.60
 H      -0.619352     2.843938     0.503986      22.96
 H      -1.804001     3.019760     1.815937      22.87
 H      -0.245177     2.720658     2.507080      21.78
 C      -0.718011    -1.040954     0.266404      30.05
 O      -2.057002    -1.202792     0.256546     200.02
 C       0.306431    -1.874700    -0.267123      43.15
 H      -0.043120    -2.848442    -0.656498      15.38
 C       2.057468    -0.487429     0.591764      62.83
 C       3.658364    -0.159087     0.465378      67.29
 H       3.942185    -0.650374    -0.363167      27.10
 O       3.803478     1.327842     0.214842     227.06
 H       3.483616     1.842343     0.980528      26.18
 C       4.443591    -0.736313     1.747514      86.26
 H       4.125011    -0.264912     2.721667      24.02
 O       4.165527    -2.341567     1.344528     207.06
 H       4.145049    -2.714945     2.206069      27.05
 C       5.933744    -0.635177     1.524071      97.28
 O       6.454181     0.848040     1.639357     205.88
 H       6.523622     1.018764     2.676050      23.57
 H       6.218209    -0.892889     0.481941      31.53
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 H       6.351638    -1.518066     1.988981      31.80
55
name= lig-ACN-Water-frame_966
 C      -4.353959    -0.495212    -3.620292      42.34
 H      -4.475425    -1.502979    -3.882004      21.70
 C      -3.820730     1.032734    -1.733746      47.12
 H      -3.901000     1.389925    -0.769306      21.18
 C      -3.779361     2.032027    -2.829473     -27.98
 O      -3.893721     3.409192    -2.545305     165.35
 C      -2.946479     3.768722    -1.482301     118.69
 H      -2.732184     4.788345    -1.847124      25.25
 H      -1.857987     3.595448    -1.760826      24.83
 H      -3.153879     4.063337    -0.272527      22.92
 C      -4.067548     1.787793    -4.277835     -37.67
 O      -3.958113     2.836585    -5.206346     174.73
 H      -4.294174     3.664024    -4.882188      22.48
 C      -4.575409     0.452393    -4.685485      33.72
 H      -4.743757     0.226632    -5.791967      31.59
 C      -3.966055    -0.261325    -2.246874      39.21
 C      -3.983915    -1.372862    -1.199242     107.66
 H      -4.440959    -2.168730    -1.732966      25.53
 O      -4.961349    -1.124879    -0.062087     157.72
 H      -4.384533    -0.639661     0.727455      22.03
 C      -2.707380    -2.107232    -0.827362      81.81
 H      -1.840205    -2.146410    -1.478973      25.15
 C      -2.963014    -3.438116    -0.054867     104.38
 O      -3.947804    -4.365343    -0.793501     239.18
 H      -3.724133    -4.467278    -1.749580      31.11
 H      -3.402293    -3.240636     0.896668      27.88
 H      -1.937336    -3.818915     0.070133      26.16
 C       1.544754    -1.586405    -0.290495      23.36
 H       2.397726    -2.261490    -0.622302      22.94
 C       1.119574     0.382196     1.396669      49.91
 H       1.243117     1.485813     1.939159      12.28
 C      -0.176633     0.039844     1.119882       2.69
 O      -1.245679     1.007951     1.453759     195.67
 C      -0.863925     2.401006     1.546377      87.60
 H       0.008746     2.546548     0.706081      22.34
 H      -1.874858     3.049090     1.718432      22.39
 H      -0.066234     2.383282     2.328615      22.61
 C      -0.700485    -1.053959     0.250761      12.10
 O      -2.025303    -1.344754     0.241057     207.63
 C       0.136274    -1.865834    -0.459146      72.28
 H      -0.077589    -2.989630    -0.812761      20.66
 C       2.017560    -0.453401     0.581249      30.75
 C       3.471410    -0.153528     0.458754      95.12
 H       3.910884    -0.506796    -0.350040      28.67
 O       3.892454     1.261149     0.316094     220.84
 H       3.631133     1.730367     1.149961      26.54
 C       4.324269    -0.861106     1.599926     105.17
 H       3.889443    -0.751846     2.663051      24.85
 O       4.233040    -2.247978     1.475438     270.11
 H       3.963668    -2.803310     2.371535      26.59
 C       5.957976    -0.629083     1.517501      95.35
 O       6.448395     0.763937     1.631251     221.59
 H       6.472384     1.128171     2.610239      23.62
 H       6.033128    -0.782447     0.478563      30.83
 H       6.693850    -1.133771     2.166184      30.17
55
name= lig-ACN-Water-frame_967
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 C      -4.322345    -0.535678    -3.602649      35.77
 H      -4.571666    -1.543592    -3.801084      27.09
 C      -3.959785     1.078495    -1.876008      58.02
 H      -3.849399     1.252777    -0.897982      12.32
 C      -3.923414     1.998277    -2.860091      27.32
 O      -3.784025     3.324529    -2.543918     239.06
 C      -3.010742     3.918600    -1.536945     103.78
 H      -3.019310     4.990970    -1.528341      24.44
 H      -2.145530     3.211826    -1.466207      22.86
 H      -3.586120     3.366127    -0.456156      20.47
 C      -4.113012     1.736131    -4.207047      34.99
 O      -3.865840     2.653008    -5.213685     185.15
 H      -4.165687     3.619236    -5.026264      23.52
 C      -4.440076     0.473079    -4.547046      82.88
 H      -4.869238     0.228757    -5.601460      21.00
 C      -3.877714    -0.282396    -2.243872      -7.45
 C      -4.068785    -1.432844    -1.308982     100.51
 H      -4.638085    -2.200155    -1.760631      28.11
 O      -4.814400    -1.039092    -0.089269     166.10
 H      -4.115056    -0.680204     0.733671      16.11
 C      -2.646262    -2.040679    -0.752222     120.89
 H      -2.216756    -2.299318    -1.721497      23.69
 C      -3.203543    -3.392916    -0.168551     114.28
 O      -3.968308    -4.441646    -0.771919     302.42
 H      -3.489514    -4.673919    -1.466145      38.10
 H      -3.667774    -3.192651     0.773391      28.55
 H      -2.293273    -3.962716     0.032982      26.04
 C       1.535130    -1.634845    -0.204345      39.74
 H       2.375353    -2.257472    -0.756933      18.07
 C       1.177910     0.352283     1.311256      55.04
 H       1.694579     1.330134     1.837695      13.88
 C      -0.292334     0.096599     1.157811       3.38
 O      -1.341475     0.974675     1.378238     167.39
 C      -0.768552     2.395174     1.567210      89.50
 H      -0.340936     2.823126     0.483843      19.19
 H      -1.847433     2.984596     1.372005      20.59
 H      -0.534866     2.772444     2.537923      23.28
 C      -0.682054    -1.036846     0.299628       7.16
 O      -2.071741    -1.352566     0.330147     242.38
 C       0.217585    -1.901695    -0.508801      48.49
 H      -0.301596    -2.525272    -1.456465      15.00
 C       1.973203    -0.434692     0.519243      24.27
 C       3.500661    -0.166009     0.482449      92.51
 H       3.655350    -0.513624    -0.415674      24.57
 O       3.907957     1.192868     0.435111     231.14
 H       4.042086     1.585191     1.357112      23.80
 C       4.320286    -0.881001     1.593029      80.57
 H       3.927178    -0.289823     2.516198      24.28
 O       4.268907    -2.319047     1.552021     278.63
 H       4.052412    -2.717649     2.527512      23.93
 C       5.890450    -0.550408     1.442795     107.81
 O       6.436493     0.715592     1.587218     256.02
 H       6.181267     0.972273     2.510584      31.08
 H       6.379002    -1.017808     0.679460      31.24
 H       6.004298    -1.294948     2.286936      29.59
55
name= lig-ACN-Water-frame_968
 C      -4.268937    -0.697290    -3.588022      64.45
 H      -4.483023    -1.709984    -3.933474      22.29
 C      -3.962439     1.020388    -1.900476      62.73
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 H      -3.785885     1.343546    -0.921913      21.95
 C      -4.040622     2.103723    -2.836643      -1.06
 O      -3.746119     3.454472    -2.686044     199.73
 C      -3.051556     3.853695    -1.398064     112.32
 H      -3.011987     4.916015    -1.593337      24.44
 H      -1.982691     3.733654    -1.276875      25.01
 H      -3.867352     3.785436    -0.380592      21.32
 C      -4.130095     1.767178    -4.183883     -22.09
 O      -3.804076     2.536167    -5.275464     104.13
 H      -3.837651     3.478587    -4.897061      22.03
 C      -4.325703     0.359394    -4.482811      25.24
 H      -4.486304     0.218896    -5.624948      22.44
 C      -4.040142    -0.331587    -2.302021      40.17
 C      -4.044297    -1.412274    -1.240454     121.83
 H      -4.586503    -2.241197    -1.658883      23.87
 O      -4.742240    -1.005898    -0.154707     233.53
 H      -4.277386    -0.168998     0.395581      18.54
 C      -2.855056    -2.127235    -0.859749      51.90
 H      -1.958980    -2.060732    -1.459547      23.19
 C      -3.208995    -3.514797    -0.043673     105.15
 O      -4.038319    -4.457949    -0.838575     223.27
 H      -3.403410    -5.007801    -1.524354      27.60
 H      -3.968050    -3.103877     0.604994      25.68
 H      -2.368642    -3.847654     0.535744      26.44
 C       1.600789    -1.600319    -0.181791      29.08
 H       2.358760    -2.116353    -0.915944      16.50
 C       0.989575     0.303006     1.113377      74.65
 H       1.456838     1.220622     1.651266      14.35
 C      -0.318421     0.049787     1.019065      19.52
 O      -1.311839     1.040442     1.396792     219.19
 C      -0.932262     2.415805     1.507408      96.09
 H       0.163283     2.538736     0.919649      19.12
 H      -1.900965     3.146298     1.380807      20.58
 H      -0.437754     2.399400     2.456598      23.07
 C      -0.732643    -1.095591     0.331732      22.96
 O      -2.084241    -1.274217     0.396166     155.60
 C       0.236332    -1.755587    -0.350799      79.62
 H      -0.002427    -2.463978    -1.364168      18.24
 C       2.047816    -0.550703     0.508272      66.95
 C       3.557085    -0.267477     0.401394      98.27
 H       4.086029    -0.602463    -0.355865      23.45
 O       3.888936     1.185098     0.519643     237.68
 H       3.914618     1.416132     1.520292      20.69
 C       4.364786    -0.774698     1.554630     106.39
 H       4.118177    -0.545598     2.651467      21.35
 O       4.257684    -2.412163     1.604681     242.41
 H       4.216413    -2.756788     2.456635      30.43
 C       5.822424    -0.741367     1.473220     107.90
 O       6.384990     0.773777     1.547825     129.14
 H       6.572253     1.089850     2.439588      30.83
 H       6.091514    -1.087404     0.589312      36.21
 H       6.468998    -1.097045     2.335025      32.65
55
name= lig-ACN-Water-frame_969
 C      -4.260190    -0.786157    -3.674979      21.02
 H      -4.056860    -1.868415    -3.928925      19.34
 C      -3.937038     1.051919    -1.891386      31.59
 H      -3.731709     1.181902    -0.799722      21.29
 C      -4.059938     2.124782    -2.860475     -13.59
 O      -3.674849     3.619882    -2.706745     140.32
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 C      -3.146824     3.961163    -1.339356      96.90
 H      -2.974978     5.065417    -1.313207      24.35
 H      -2.303334     3.297838    -1.301118      25.77
 H      -3.711725     3.578235    -0.231149      21.70
 C      -4.105002     1.624313    -4.238705     -27.57
 O      -3.780472     2.502403    -5.318222     169.33
 H      -3.638444     3.417146    -5.172482      22.99
 C      -4.250147     0.260217    -4.638339      54.92
 H      -3.973550    -0.018170    -5.678814      26.39
 C      -4.170726    -0.334538    -2.258898       4.66
 C      -4.081421    -1.433225    -1.238603      96.32
 H      -4.730669    -2.165890    -1.693377      23.58
 O      -4.885484    -0.974938    -0.098932     202.65
 H      -4.389803    -0.373245     0.627953      20.56
 C      -2.759414    -2.300474    -0.740556      68.49
 H      -2.177219    -2.586098    -1.640086      20.11
 C      -3.256467    -3.518505     0.033528     101.66
 O      -4.050739    -4.473989    -0.870507     185.71
 H      -3.318359    -4.856967    -1.669722      25.31
 H      -4.032281    -3.270923     0.781236      25.20
 H      -2.446562    -3.994087     0.562500      25.83
 C       1.639345    -1.608936    -0.275245      38.19
 H       2.282707    -2.364067    -0.776138      22.25
 C       1.115228     0.341183     0.966254      67.79
 H       1.177165     1.292939     1.456838      15.64
 C      -0.378906     0.117663     0.892837       6.38
 O      -1.338994     1.003445     1.384585     207.86
 C      -0.927709     2.388318     1.574003      96.29
 H      -0.225165     2.804264     0.592727      20.52
 H      -1.912679     3.054524     1.230758      21.19
 H      -0.750329     2.803897     2.559391      23.93
 C      -0.868760    -1.097750     0.375063      14.08
 O      -2.238798    -1.285575     0.323597     163.96
 C       0.192119    -1.835238    -0.316276      81.07
 H      -0.210827    -2.963050    -0.651830      19.34
 C       2.151999    -0.531797     0.534483      18.21
 C       3.664207    -0.208190     0.479814      75.14
 H       3.800080    -0.538042    -0.448465      25.01
 O       3.811368     1.171342     0.498026     303.65
 H       3.688273     1.540558     1.425313      22.77
 C       4.382589    -1.046483     1.735068      96.42
 H       3.729579    -0.531696     2.498833      23.19
 O       4.233871    -2.354926     1.555097     353.18
 H       4.079997    -2.845214     2.335479      30.22
 C       5.994822    -0.693581     1.506869     101.84
 O       6.314793     0.747332     1.464115     200.45
 H       6.361406     0.945856     2.442353      27.46
 H       6.184565    -1.029395     0.616163      36.98
 H       6.580452    -1.486648     2.165801      31.86
55
name= lig-ACN-Water-frame_970
 C      -4.206890    -0.681911    -3.654562      59.21
 H      -4.123398    -1.804948    -3.850411      25.51
 C      -3.990196     1.096427    -1.955994      42.59
 H      -3.825541     1.392493    -0.828368      17.26
 C      -3.936365     2.114154    -2.928620     -35.88
 O      -3.700654     3.580364    -2.690090     180.55
 C      -3.171594     3.958746    -1.317024     102.15
 H      -2.809282     5.017390    -1.086655      23.72
 H      -2.309215     3.415204    -1.007255      23.82
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 H      -4.259552     3.709958    -0.835451      23.02
 C      -4.021100     1.592348    -4.351973     -34.08
 O      -3.783593     2.452802    -5.373790     129.59
 H      -3.929183     3.313099    -4.899120      21.53
 C      -4.096369     0.208158    -4.736350      74.10
 H      -3.927236    -0.000461    -5.758400      18.86
 C      -4.131745    -0.295146    -2.340805       7.58
 C      -4.239067    -1.549909    -1.166455      71.61
 H      -4.814555    -2.422187    -1.558882      26.01
 O      -5.094448    -1.030977    -0.015971     181.30
 H      -4.556474    -0.604629     0.579549      27.62
 C      -2.867107    -2.299174    -0.604942      86.14
 H      -2.056666    -2.550096    -1.339261      21.99
 C      -3.357813    -3.615756     0.063089     111.42
 O      -3.987453    -4.461866    -0.849144     318.34
 H      -3.532867    -4.343925    -1.761260      31.52
 H      -3.963723    -3.287677     0.992824      25.47
 H      -2.525445    -4.160457     0.415831      26.74
 C       1.465531    -1.640780    -0.222788      55.51
 H       2.150183    -2.347333    -0.586592      25.97
 C       1.142530     0.467387     0.923138      62.20
 H       1.717068     1.222754     1.236991       8.85
 C      -0.292782     0.182614     0.814373       3.95
 O      -1.330008     0.955945     1.384195     187.96
 C      -1.026708     2.445148     1.556389      83.49
 H      -0.124230     2.839828     0.779796      19.47
 H      -2.165826     2.831264     1.454761      20.52
 H      -0.553400     2.412316     2.590205      22.26
 C      -0.776515    -1.084833     0.266795       2.36
 O      -2.327018    -1.368830     0.209210     193.62
 C       0.125026    -2.039600    -0.211127      58.58
 H      -0.140261    -3.131342    -0.560080      16.32
 C       2.061861    -0.523245     0.408257      66.60
 C       3.640009    -0.239398     0.614310      88.73
 H       4.296857    -0.565648    -0.104842      20.16
 O       3.755505     1.239017     0.441536     245.16
 H       3.879816     1.601141     1.357102      23.81
 C       4.489214    -0.985736     1.773728      97.75
 H       4.417961    -0.907316     2.899256      22.64
 O       4.183259    -2.441722     1.425336     312.81
 H       3.877515    -3.043814     2.254692      23.76
 C       6.021768    -0.704632     1.503144     108.30
 O       6.293833     0.668852     1.480871     274.29
 H       6.055635     1.227473     2.279515      30.64
 H       6.305676    -1.010397     0.619179      34.50
 H       6.735981    -1.046082     2.409810      29.33
55
name= lig-ACN-Water-frame_971
 C      -4.095223    -0.682933    -3.656132      36.60
 H      -4.476480    -1.700160    -3.985486      23.97
 C      -4.043790     1.087688    -2.010744      40.17
 H      -4.160144     1.513810    -0.889412      15.34
 C      -3.789686     2.037196    -3.064194      25.04
 O      -3.704096     3.414572    -2.754699     138.55
 C      -3.296299     3.851687    -1.303546      89.19
 H      -3.102549     4.803398    -1.859211      23.20
 H      -2.496298     3.281902    -0.939258      24.24
 H      -4.010696     4.015645    -0.339706      22.97
 C      -3.851429     1.648404    -4.371149      23.89
 O      -3.810584     2.517831    -5.458330     175.65
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 H      -3.874450     3.557642    -5.380673      22.65
 C      -3.947781     0.277539    -4.695064      69.54
 H      -4.121355    -0.041254    -5.650816      18.70
 C      -4.077541    -0.341858    -2.196843       2.45
 C      -4.420429    -1.509577    -1.131121      91.15
 H      -5.081560    -2.213565    -1.757289      24.61
 O      -5.248557    -1.169130    -0.017204     206.20
 H      -4.924870    -0.406111     0.402513      27.68
 C      -3.124834    -2.258702    -0.635957      43.10
 H      -2.642011    -2.475917    -1.656353      20.16
 C      -3.306920    -3.672298     0.175581     104.14
 O      -3.998959    -4.483349    -0.893036     256.51
 H      -3.783226    -4.241007    -1.699874      36.19
 H      -4.254142    -3.697815     0.862869      23.29
 H      -2.391986    -3.941715     0.600242      26.81
 C       1.474972    -1.798695    -0.098472      47.21
 H       2.140289    -2.525389    -0.404388      23.05
 C       1.108309     0.521118     0.849799      57.82
 H       1.167450     1.381586     1.271157      14.69
 C      -0.258235     0.169621     0.776632       2.29
 O      -1.275674     0.947728     1.330022     204.66
 C      -1.119647     2.352969     1.602210      84.38
 H      -0.507685     2.811666     0.623080      19.88
 H      -2.048041     3.090043     1.699466      21.84
 H      -0.513560     2.579572     2.632224      21.37
 C      -0.850879    -1.098181     0.155815      12.43
 O      -2.140238    -1.256348     0.299802     139.45
 C       0.054946    -2.153977    -0.099835      81.11
 H      -0.260775    -3.019576    -0.678684      20.87
 C       1.959497    -0.509606     0.320049      24.27
 C       3.551681    -0.239823     0.641568      77.00
 H       3.800310    -0.706528    -0.277514      20.97
 O       3.736556     1.276401     0.441197     242.12
 H       3.723113     1.660701     1.359298      23.47
 C       4.535194    -0.966352     1.770130      89.25
 H       4.207804    -0.822399     2.809042      24.53
 O       4.159231    -2.489886     1.285723     257.31
 H       3.981917    -2.973404     2.280935      23.00
 C       6.023051    -0.799275     1.543016      99.30
 O       6.313803     0.732449     1.470564     212.10
 H       6.353612     0.887721     2.472778      26.99
 H       6.348747    -1.310250     0.725375      34.68
 H       6.556131    -1.400131     2.436643      31.18
55
name= lig-ACN-Water-frame_972
 C      -4.013795    -0.695830    -3.553941      53.43
 H      -4.167249    -1.738645    -3.895188      24.20
 C      -4.024285     0.995469    -1.995581      77.21
 H      -4.354413     1.506029    -0.999214      20.59
 C      -3.728159     1.928277    -3.003716     -14.31
 O      -3.732290     3.252212    -2.740787     216.84
 C      -3.360603     3.812783    -1.457497     101.47
 H      -2.884252     4.831824    -1.262215      23.79
 H      -2.554929     3.142921    -1.081878      24.76
 H      -4.254156     3.657308    -0.766221      24.23
 C      -3.648331     1.701628    -4.482384      -8.93
 O      -3.827328     2.616206    -5.596548     148.52
 H      -3.728975     3.526237    -5.159450      22.05
 C      -3.864958     0.301854    -4.586758      42.51
 H      -4.014932    -0.012325    -5.577769      23.95
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 C      -4.120702    -0.351125    -2.210519      42.04
 C      -4.503703    -1.389385    -1.122141      94.41
 H      -5.014827    -2.240068    -1.728841      23.59
 O      -5.412403    -1.213135    -0.012254     132.60
 H      -5.087567    -0.357873     0.590334      23.57
 C      -3.245538    -2.210198    -0.618563      41.91
 H      -2.612271    -2.549178    -1.533328      20.23
 C      -3.383162    -3.558465     0.093598     104.71
 O      -3.984940    -4.548214    -0.892040     229.21
 H      -3.342735    -4.566585    -1.653113      29.32
 H      -3.873170    -3.460297     1.181199      23.83
 H      -2.451341    -4.048507     0.294725      24.49
 C       1.510389    -1.887518     0.048033      38.64
 H       2.260706    -2.648971    -0.070336      20.81
 C       0.943510     0.447632     0.724187      93.32
 H       1.464170     1.208111     1.090870      17.52
 C      -0.382859     0.110687     0.690133      18.52
 O      -1.327919     0.935195     1.273997     194.94
 C      -1.093867     2.315720     1.627099      83.49
 H      -0.753399     3.045264     0.711493      22.60
 H      -2.216585     2.409930     1.811919      21.11
 H      -0.326807     2.496302     2.585561      21.31
 C      -0.776911    -1.088833     0.190782      14.04
 O      -2.228194    -1.169693     0.347346      97.46
 C       0.113637    -2.129891    -0.123238      41.04
 H      -0.301765    -3.029332    -0.334821      20.11
 C       1.993539    -0.548598     0.482589      50.76
 C       3.476658    -0.166957     0.442930      83.54
 H       4.042956    -0.346958    -0.476542      21.13
 O       3.722723     1.202573     0.490164     281.59
 H       3.534756     1.618467     1.377288      25.71
 C       4.286415    -1.100747     1.575712      90.95
 H       3.866436    -0.815731     2.498292      26.05
 O       4.205217    -2.399983     1.251787     303.46
 H       3.999989    -3.114356     1.965293      27.35
 C       6.000478    -0.782630     1.567959      94.80
 O       6.377972     0.633993     1.523254     234.45
 H       6.694390     1.108310     2.313982      27.76
 H       6.315273    -1.076274     0.579369      32.32
 H       6.561606    -1.275963     2.466016      29.81
55
name= lig-ACN-Water-frame_973
 C      -3.946218    -0.715906    -3.558443      50.65
 H      -3.729511    -1.736673    -3.812222      24.32
 C      -3.989611     1.021412    -1.928541      45.04
 H      -4.114563     1.356222    -0.878590      21.14
 C      -3.694953     1.939355    -3.042253     -16.12
 O      -3.743432     3.325175    -2.786308     210.72
 C      -3.363906     3.641470    -1.458948     110.75
 H      -3.357768     4.753833    -1.664768      23.51
 H      -2.440885     3.183244    -1.013391      25.85
 H      -4.284454     3.511877    -0.743288      24.07
 C      -3.596648     1.616495    -4.424507      -5.95
 O      -3.773798     2.609034    -5.560399     152.71
 H      -3.936653     3.546307    -5.315798      24.38
 C      -3.781109     0.219652    -4.649846      39.93
 H      -3.605320    -0.276398    -5.619319      22.84
 C      -4.232441    -0.365988    -2.206966      22.72
 C      -4.471174    -1.467537    -1.126268      78.74
 H      -5.065257    -2.316617    -1.638588      24.10
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 O      -5.520996    -1.085737    -0.021737     105.36
 H      -4.932376    -0.634410     0.801286      25.46
 C      -3.135817    -2.055239    -0.606682      68.23
 H      -2.413439    -1.995578    -1.512500      21.49
 C      -3.420604    -3.502947    -0.047229      98.22
 O      -3.981336    -4.560016    -0.804432     212.87
 H      -3.148409    -4.931071    -1.513358      24.17
 H      -4.130011    -3.517388     0.925277      23.48
 H      -2.363049    -3.610689     0.233765      23.93
 C       1.550628    -1.887209     0.206561      53.26
 H       2.234946    -2.777069     0.105165      16.74
 C       1.046553     0.356783     0.656062      76.36
 H       1.087494     1.415109     0.724833      16.06
 C      -0.435477     0.170192     0.665383       6.47
 O      -1.444986     0.914007     1.201240     173.49
 C      -1.137843     2.296026     1.662983      88.33
 H      -0.796300     2.872542     0.712967      24.70
 H      -1.830147     2.901721     2.220803      24.28
 H      -0.084461     2.061023     2.351517      22.26
 C      -0.923113    -1.177900     0.242010      -7.67
 O      -2.434451    -1.226233     0.287795     167.13
 C       0.175931    -2.105042    -0.118945      51.47
 H       0.030158    -3.058485    -0.261460      21.93
 C       1.934153    -0.657760     0.509065      31.86
 C       3.489843    -0.230721     0.295778      77.80
 H       3.806625    -0.585235    -0.734364      21.29
 O       3.692201     1.215422     0.571382     271.49
 H       3.725856     1.308663     1.566206      24.32
 C       4.212391    -0.960596     1.393770     105.69
 H       3.763983    -0.837468     2.300714      25.56
 O       4.234267    -2.478297     1.162019     287.71
 H       3.903917    -2.743427     1.940976      31.56
 C       5.800422    -0.689815     1.536083      95.33
 O       6.486065     0.550133     1.540916     317.93
 H       6.308036     0.851402     2.399664      32.30
 H       6.207067    -1.359877     0.725399      28.99
 H       6.176546    -1.391586     2.391587      28.67
55
name= lig-ACN-Water-frame_974
 C      -3.892535    -0.758485    -3.623899      67.25
 H      -3.920742    -1.811032    -3.802656      29.36
 C      -3.977350     1.040779    -1.959675      56.71
 H      -3.893973     1.419430    -1.008787      22.18
 C      -3.753840     1.985243    -3.046172       1.17
 O      -3.705803     3.351861    -2.870470     200.78
 C      -3.420384     3.661317    -1.368045      95.86
 H      -3.098545     4.730650    -1.282961      24.12
 H      -2.364329     3.164523    -1.276197      23.21
 H      -4.137766     3.385095    -0.567628      25.39
 C      -3.747028     1.530653    -4.397072       4.06
 O      -3.655624     2.440618    -5.395452     103.56
 H      -3.941451     3.295771    -5.018160      22.88
 C      -3.626818     0.088012    -4.701236      55.17
 H      -3.275856    -0.209138    -5.765108      15.20
 C      -4.257666    -0.312830    -2.234468      12.18
 C      -4.518693    -1.435762    -1.141124      83.74
 H      -4.934633    -2.389803    -1.646676      24.97
 O      -5.451345    -0.949107    -0.090904     186.27
 H      -4.943285    -0.681119     0.640633      28.13
 C      -3.113869    -2.005060    -0.794540      63.73
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 H      -2.605570    -2.255008    -1.787458      21.91
 C      -3.304412    -3.454490    -0.047519      96.62
 O      -3.956007    -4.571621    -0.752676     223.36
 H      -3.480945    -4.965756    -1.631934      26.77
 H      -4.153942    -3.067767     0.641563      25.13
 H      -2.610049    -3.990734     0.690404      24.31
 C       1.421807    -1.965052     0.252424      23.57
 H       2.213384    -2.802275     0.138246      15.51
 C       0.911963     0.468407     0.636620      64.86
 H       1.518880     1.435276     0.608784      14.04
 C      -0.492061     0.011143     0.669026      -0.75
 O      -1.568918     0.975458     1.118450     134.27
 C      -1.040265     2.216359     1.669656     100.18
 H      -0.869792     2.992097     0.828523      23.49
 H      -1.919264     2.399483     2.182073      23.74
 H       0.017723     2.297335     2.412470      22.50
 C      -1.022335    -1.179327     0.285586       9.40
 O      -2.452272    -1.266407     0.307305     205.80
 C       0.009241    -2.198260     0.013916      46.43
 H      -0.310321    -2.970740    -0.528811      21.63
 C       2.004844    -0.549091     0.395683      14.53
 C       3.409086    -0.244153     0.295908      92.50
 H       3.703275    -0.208307    -0.848840      22.88
 O       3.650515     1.186181     0.598102     252.41
 H       3.908715     1.368801     1.537362      27.37
 C       4.265329    -0.892409     1.299739     107.78
 H       3.821946    -0.589388     2.150422      26.62
 O       4.220928    -2.494730     1.080496     208.81
 H       3.871420    -3.056348     1.839072      27.16
 C       5.690782    -0.782669     1.471288     102.57
 O       6.527315     0.480384     1.499234     243.45
 H       6.741163     0.946677     2.282046      31.48
 H       6.247819    -1.345518     0.606570      28.42
 H       5.737135    -1.204243     2.520290      29.57
55
name= lig-ACN-Water-frame_975
 C      -3.936750    -0.844735    -3.607595      76.70
 H      -4.085870    -1.887369    -3.831402      23.21
 C      -4.003054     1.025873    -2.003733      77.65
 H      -4.093608     1.240895    -1.018490      23.14
 C      -3.899173     1.915808    -3.043764     -12.35
 O      -3.672144     3.414673    -2.788882     186.52
 C      -3.344759     3.726518    -1.415247     109.37
 H      -3.374403     4.774523    -1.185721      25.78
 H      -2.412908     3.191167    -1.008536      26.06
 H      -4.191703     3.252996    -0.881882      25.44
 C      -3.831610     1.372133    -4.354215      24.55
 O      -3.548204     2.314404    -5.301581     171.81
 H      -3.632110     3.279847    -4.972244      21.20
 C      -3.515978     0.086939    -4.620235      63.34
 H      -3.249475    -0.297333    -5.711556      19.88
 C      -4.167404    -0.326884    -2.399234      39.65
 C      -4.507597    -1.289527    -1.282634      77.93
 H      -5.269130    -2.023789    -1.735982      23.32
 O      -5.302992    -0.882262    -0.170321     221.62
 H      -4.841627    -0.299635     0.382903      28.88
 C      -3.124017    -2.218734    -0.863120      32.36
 H      -2.340156    -1.974339    -1.622237      22.09
 C      -3.337869    -3.424253    -0.000098     102.77
 O      -3.941084    -4.561268    -0.736830     289.06
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 H      -3.532488    -4.436270    -1.505838      33.70
 H      -4.065134    -3.142876     0.817856      24.90
 H      -2.202962    -3.562078     0.411912      22.99
 C       1.219361    -1.866601     0.169781      60.56
 H       1.917945    -2.706208    -0.016036      20.00
 C       0.800029     0.418018     0.566371      79.06
 H       0.884024     1.490086     0.961571      15.86
 C      -0.530531     0.140555     0.743977      19.45
 O      -1.479440     0.981217     1.006666     231.43
 C      -1.070362     2.213702     1.683215     108.12
 H      -0.886675     3.030071     0.967205      25.40
 H      -1.708025     2.631772     2.392186      27.06
 H      -0.024882     1.752357     2.314353      22.58
 C      -1.011555    -1.229373     0.323918      15.21
 O      -2.358505    -1.278714     0.270848     159.48
 C      -0.162345    -2.274767     0.141877      51.77
 H      -0.409589    -3.273768    -0.157594      19.57
 C       1.646867    -0.605452     0.317776      36.92
 C       3.370521    -0.079229     0.240449      68.28
 H       3.960965    -0.416105    -0.735543      20.98
 O       3.607757     1.231874     0.584780     270.35
 H       3.667996     1.268045     1.581316      24.08
 C       4.168225    -1.092390     1.306893      96.76
 H       3.743308    -0.951969     2.222826      25.40
 O       4.174248    -2.402379     1.007197     272.66
 H       3.818456    -2.857072     1.965572      23.79
 C       5.924131    -0.845483     1.486956      77.44
 O       6.524479     0.424173     1.374160     285.81
 H       6.341824     0.723499     2.282247      29.03
 H       6.329733    -1.629291     0.627528      28.05
 H       6.284106    -1.408000     2.367965      29.46
55
name= lig-ACN-Water-frame_976
 C      -3.946883    -0.950494    -3.708515      50.70
 H      -3.928412    -2.036479    -3.901430      19.39
 C      -4.097032     0.973997    -1.994676      75.51
 H      -4.204123     1.265971    -0.958644      21.65
 C      -3.991063     2.011674    -2.967182      23.08
 O      -3.637773     3.323218    -2.789810     210.38
 C      -3.374337     3.716830    -1.410868     122.88
 H      -3.155325     4.740006    -1.652167      25.13
 H      -2.276879     3.509249    -1.047712      25.50
 H      -4.070474     3.587863    -0.619799      26.57
 C      -3.710728     1.471796    -4.273080     -10.02
 O      -3.456344     2.281282    -5.368182     121.31
 H      -3.738359     3.243260    -5.140821      22.53
 C      -3.556551    -0.012225    -4.597110      46.50
 H      -3.202867    -0.265463    -5.686619      22.55
 C      -4.097876    -0.367330    -2.329575      20.69
 C      -4.432554    -1.389072    -1.367243      91.54
 H      -5.118269    -2.107108    -1.892021      26.13
 O      -5.145846    -0.797555    -0.211840     173.59
 H      -4.560556    -0.052567     0.301109      21.07
 C      -3.133551    -2.123842    -0.774347      76.77
 H      -2.615501    -2.727283    -1.573484      20.25
 C      -3.388933    -3.444446     0.012895      96.17
 O      -3.892479    -4.508631    -0.727988     279.61
 H      -3.752372    -4.492042    -1.672988      32.28
 H      -3.880516    -3.337311     0.980767      25.63
 H      -2.278020    -3.954207     0.352892      21.82
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 C       1.124334    -1.945972    -0.015675      37.95
 H       1.880689    -2.648827    -0.204012      19.77
 C       0.734346     0.476972     0.596725      80.60
 H       1.306520     1.455699     0.579241      14.93
 C      -0.637652     0.039046     0.666756       8.23
 O      -1.560019     1.123464     0.966940     174.94
 C      -1.059318     2.223846     1.733878     102.73
 H      -0.628249     2.962450     1.065039      24.95
 H      -1.961892     2.417947     2.226209      25.27
 H      -0.067338     2.055223     2.626354      22.27
 C      -1.099618    -1.196620     0.411238      24.45
 O      -2.456421    -1.299168     0.170980     212.56
 C      -0.203499    -2.299228     0.223703      50.91
 H      -0.509289    -3.379968     0.475830      18.01
 C       1.660786    -0.546327     0.207305      20.93
 C       3.300612    -0.227869     0.321533      57.20
 H       3.493306    -0.205008    -0.892759      20.74
 O       3.539489     1.328582     0.583548     226.83
 H       3.424504     1.456569     1.567238      27.03
 C       4.251196    -1.048285     1.401926      85.20
 H       3.814677    -0.905955     2.347885      26.44
 O       4.063746    -2.489405     0.922927     265.50
 H       3.751760    -3.161211     1.656067      27.18
 C       5.998387    -0.989431     1.424995      74.55
 O       6.522707     0.398659     1.282588     200.05
 H       6.284138     1.188778     1.939362      26.44
 H       6.369027    -1.426659     0.310057      24.96
 H       6.269012    -1.444474     2.351859      29.62
55
name= lig-ACN-Water-frame_977
 C      -3.887470    -0.882846    -3.643572      65.01
 H      -3.907700    -1.968345    -3.909372      27.63
 C      -4.202571     0.962303    -2.002293      53.96
 H      -4.322276     1.298457    -0.892737      15.64
 C      -3.904981     1.879418    -2.996194       1.84
 O      -3.660937     3.234375    -2.762234     215.41
 C      -3.304931     3.864123    -1.422038     106.50
 H      -3.158562     4.905485    -1.438677      24.39
 H      -2.493716     3.089598    -1.269146      24.59
 H      -4.089444     3.615528    -0.684044      23.83
 C      -3.541654     1.448267    -4.322073      18.23
 O      -3.393751     2.306920    -5.463118     215.93
 H      -3.743172     3.207399    -5.339275      30.38
 C      -3.668818     0.156970    -4.664944      52.10
 H      -3.340598    -0.095074    -5.705503      19.10
 C      -4.097964    -0.489502    -2.388166      15.44
 C      -4.351567    -1.532638    -1.178064     104.35
 H      -4.969615    -2.406594    -1.423808      24.65
 O      -5.063603    -0.782422    -0.248254     199.30
 H      -4.320168    -0.372736     0.473955      19.38
 C      -3.152844    -2.222007    -0.697444      80.39
 H      -2.392299    -2.096430    -1.569831      17.70
 C      -3.363148    -3.512330     0.089563      98.59
 O      -3.974978    -4.547731    -0.775891     217.03
 H      -3.450156    -4.259569    -1.752607      24.51
 H      -4.155766    -3.334812     0.826092      25.20
 H      -2.265029    -3.725880     0.622840      22.74
 C       1.225435    -1.915821    -0.100786      43.10
 H       1.790752    -2.760230    -0.243469      20.02
 C       0.795986     0.397496     0.554671      34.47
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 H       0.947864     1.448072     0.672406      14.49
 C      -0.697476     0.207315     0.611432     -19.87
 O      -1.652983     1.162086     0.927789     171.01
 C      -1.071491     2.310027     1.799348      82.22
 H      -0.644567     3.092689     1.221081      22.77
 H      -1.894927     2.898775     2.229642      23.67
 H      -0.436539     1.709514     2.769611      21.01
 C      -1.239760    -1.246761     0.391574      -5.38
 O      -2.609915    -1.218445     0.141583     178.49
 C      -0.185108    -2.227863     0.280698      53.77
 H      -0.594411    -3.382044     0.205557      18.03
 C       1.762085    -0.620568     0.207604      31.09
 C       3.231915    -0.214911     0.414709      76.82
 H       4.016379    -0.453824    -0.546650      19.39
 O       3.425670     1.266559     0.573927     248.46
 H       3.400526     1.546462     1.527151      26.10
 C       4.322823    -1.077278     1.341591      84.16
 H       4.175662    -0.854317     2.397621      24.94
 O       3.962281    -2.578121     0.874952     242.91
 H       3.742324    -3.025057     1.618516      28.59
 C       5.822161    -0.918939     1.289209      97.41
 O       6.547645     0.360769     1.189480     232.55
 H       6.245549     0.726480     2.088120      29.93
 H       6.323273    -1.692472     0.408142      26.21
 H       6.243299    -1.431374     2.111326      30.31
55
name= lig-ACN-Water-frame_978
 C      -3.800438    -0.766765    -3.706384      47.40
 H      -3.809738    -1.793102    -4.128467      24.52
 C      -4.222257     0.795161    -2.070721      37.86
 H      -4.615139     1.264323    -1.042304      15.81
 C      -3.686354     1.813639    -3.019634       0.93
 O      -3.733058     3.280174    -2.762019     189.10
 C      -3.252421     3.782289    -1.455045     115.75
 H      -2.909558     4.759516    -1.761099      24.11
 H      -2.338487     3.545795    -0.741634      22.78
 H      -4.133649     3.814773    -0.782450      23.95
 C      -3.527282     1.525264    -4.444323      -0.96
 O      -3.343592     2.370068    -5.504680     129.39
 H      -3.486691     3.256749    -5.138297      23.79
 C      -3.721806     0.140979    -4.743289      43.43
 H      -3.840953    -0.239746    -5.737099      21.12
 C      -4.180795    -0.543701    -2.265796      36.36
 C      -4.438866    -1.585443    -1.213413      87.37
 H      -5.199041    -2.212079    -1.631422      21.89
 O      -5.095244    -0.841221    -0.134205     225.91
 H      -4.542588    -0.361279     0.534991      21.09
 C      -3.045873    -2.302910    -0.656484      58.46
 H      -2.326444    -2.645736    -1.492378      19.26
 C      -3.430954    -3.585787     0.117604      92.97
 O      -3.989693    -4.554900    -0.831181     214.00
 H      -3.367427    -4.739113    -1.772924      24.95
 H      -4.141193    -3.303269     0.864309      25.47
 H      -2.530167    -4.173339     0.820383      22.02
 C       1.207013    -1.908086     0.023951      34.62
 H       1.852876    -2.687027    -0.307339      19.44
 C       0.697623     0.341391     0.518013      90.76
 H       1.160586     1.153886     0.894246      17.82
 C      -0.664913     0.181634     0.550899      16.76
 O      -1.622985     1.228375     0.922324     183.27
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 C      -1.187811     2.342130     1.808891      87.27
 H      -0.362561     2.793052     1.343451      22.69
 H      -2.158427     2.880122     2.095834      20.90
 H      -0.528524     1.744909     2.805845      21.50
 C      -1.155304    -1.015657     0.342675      20.70
 O      -2.589200    -1.122933     0.295707     160.96
 C      -0.198255    -2.093622     0.150389      56.10
 H      -0.366437    -3.191475    -0.392344      16.84
 C       1.762864    -0.653787     0.315970      18.96
 C       3.379234    -0.210987     0.394069      69.12
 H       3.597305    -0.364308    -0.846598      18.95
 O       3.327584     1.146263     0.584630     326.52
 H       3.341568     1.318523     1.555779      27.11
 C       4.129999    -1.168354     1.281123     103.45
 H       3.740776    -1.233982     2.308049      23.91
 O       3.943296    -2.508893     0.924641     288.23
 H       3.633763    -3.018582     1.764615      26.31
 C       5.775806    -0.950678     1.099276      85.08
 O       6.498849     0.307923     1.161319     245.40
 H       6.584331     0.731536     1.971854      32.45
 H       6.059882    -1.500397    -0.011860      25.82
 H       6.072530    -1.479167     1.963594      28.10
55
name= lig-ACN-Water-frame_979
 C      -3.837549    -0.894033    -3.717218      44.86
 H      -3.745589    -1.950987    -3.938243      24.32
 C      -4.127956     0.913604    -2.150146      42.47
 H      -4.657322     1.262869    -1.154947      21.65
 C      -3.603463     1.845608    -3.051223     -13.32
 O      -3.739165     3.189485    -2.757459     135.32
 C      -3.232494     3.804564    -1.475945      98.50
 H      -2.787953     4.787127    -1.722685      23.48
 H      -2.500191     2.861393    -1.263858      21.28
 H      -4.063704     4.080763    -0.723619      22.39
 C      -3.594407     1.521506    -4.461442      -5.14
 O      -3.295016     2.480116    -5.481016     100.39
 H      -3.543890     3.474368    -5.355501      20.08
 C      -3.722660     0.135006    -4.794950      52.56
 H      -3.756834    -0.152685    -5.804515      20.67
 C      -4.113729    -0.533231    -2.423011      19.98
 C      -4.481329    -1.551026    -1.237185      83.59
 H      -4.980068    -2.440460    -1.496256      26.46
 O      -5.226428    -1.017030    -0.008653     199.14
 H      -4.707061    -0.388301     0.338965      29.27
 C      -3.106878    -2.241223    -0.549511      61.16
 H      -2.289906    -2.416313    -1.301524      21.58
 C      -3.521571    -3.650360     0.116888      90.77
 O      -4.010642    -4.570724    -0.852332     268.01
 H      -3.310534    -4.649134    -1.493012      31.57
 H      -4.338585    -3.621137     0.803330      25.32
 H      -2.358769    -4.072002     0.565826      22.04
 C       1.149911    -1.918090     0.147939      48.06
 H       1.757744    -2.810538    -0.139331      19.75
 C       0.825866     0.479407     0.617952      51.75
 H       1.157886     1.445034     0.710469      16.17
 C      -0.619042     0.326583     0.604636       9.30
 O      -1.551631     1.267049     0.895725     228.37
 C      -1.203806     2.253044     1.795802     122.57
 H      -0.666178     3.150612     1.435477      23.99
 H      -2.219045     2.915714     1.780739      22.74
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 H      -1.131785     2.080778     3.015465      23.57
 C      -1.141207    -1.021580     0.231777       9.61
 O      -2.452064    -1.238169     0.362865     230.91
 C      -0.229657    -2.008513    -0.141767      71.05
 H      -0.961089    -2.955780    -0.326949      17.39
 C       1.706498    -0.646094     0.408818      40.58
 C       3.144930    -0.336052     0.224411      64.38
 H       3.753973    -0.343325    -0.900333      20.30
 O       3.342023     1.120248     0.654352     240.65
 H       3.539747     1.289357     1.624956      26.50
 C       4.074751    -1.133435     1.268422      80.82
 H       3.818779    -0.527057     2.184393      24.60
 O       3.937333    -2.534297     0.949442     251.27
 H       3.484943    -3.245001     1.716722      25.10
 C       5.689355    -1.037471     1.062516      85.97
 O       6.427102     0.266583     1.133990     209.95
 H       6.267221     0.533213     2.098116      30.57
 H       5.813725    -1.177149    -0.158458      26.24
 H       6.276409    -1.899263     1.352950      29.08
55
name= lig-ACN-Water-frame_980
 C      -3.897504    -0.958202    -3.846334      49.28
 H      -3.893261    -1.987838    -4.149975      24.04
 C      -4.011226     0.911011    -2.154021      87.95
 H      -4.192071     1.330333    -1.123596      22.19
 C      -3.734765     1.884181    -3.143644     -20.44
 O      -3.757984     3.248479    -2.791573     175.97
 C      -3.168703     3.731833    -1.547979      88.44
 H      -2.465866     4.610901    -1.718575      23.50
 H      -2.430387     3.013299    -0.824961      21.91
 H      -4.093787     3.780882    -0.792636      21.84
 C      -3.592185     1.491314    -4.474118      12.17
 O      -3.263089     2.484992    -5.421338      73.21
 H      -3.850888     3.289049    -5.212952      19.79
 C      -3.683499     0.103410    -4.770148      55.56
 H      -3.324238    -0.144090    -5.751328      20.63
 C      -4.091015    -0.425400    -2.441341     -38.20
 C      -4.395870    -1.500806    -1.093776      93.23
 H      -4.909835    -2.200628    -1.703641      26.36
 O      -5.356994    -1.208202    -0.045458     184.92
 H      -4.997405    -0.764468     0.722624      25.74
 C      -3.245534    -2.147373    -0.525891      90.18
 H      -2.715880    -2.348968    -1.481108      22.64
 C      -3.541039    -3.602399     0.101796      78.62
 O      -4.015860    -4.595615    -0.890838     315.93
 H      -3.592471    -4.517125    -1.661301      33.97
 H      -4.208433    -3.484017     0.965462      24.40
 H      -2.451947    -3.979732     0.742387      22.84
 C       1.058783    -1.917049     0.090644      30.95
 H       1.800064    -2.791051     0.185352      14.13
 C       0.828804     0.608204     0.719931      94.75
 H       1.306483     1.633554     0.643496      13.51
 C      -0.503418     0.285748     0.625466      22.17
 O      -1.499507     1.253452     0.842257     158.93
 C      -1.336226     2.441891     1.840092      92.95
 H      -0.306615     2.824618     1.667752      23.30
 H      -2.379038     3.039188     1.814188      21.98
 H      -1.043873     1.677451     2.756514      23.43
 C      -1.058693    -0.933288     0.138571      13.97
 O      -2.446927    -1.395083     0.415499     222.00
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 C      -0.273432    -2.009292    -0.297380      52.23
 H      -0.418532    -3.143148    -0.472670      17.05
 C       1.586116    -0.624768     0.417322      30.50
 C       3.100036    -0.277403     0.319638      62.81
 H       3.271220    -0.579446    -0.934218      18.40
 O       3.406104     1.072062     0.636117     256.77
 H       3.667378     1.014380     1.603781      25.66
 C       4.148421    -1.099529     1.190190     100.11
 H       3.878878    -1.209272     2.355768      22.31
 O       3.895599    -2.632733     1.006484     240.55
 H       3.562864    -2.874692     1.934947      25.33
 C       5.593157    -1.021126     0.838001      90.50
 O       6.310703     0.156124     1.216067     252.57
 H       6.018344     0.671744     2.078573      30.78
 H       5.585995    -1.201225    -0.340404      27.02
 H       5.999431    -1.830241     1.473294      28.75
55
name= lig-ACN-Water-frame_981
 C      -3.981949    -0.810943    -3.782088      43.17
 H      -4.092862    -1.826590    -4.126657      23.91
 C      -3.908621     0.918433    -2.104946      39.18
 H      -3.738082     1.121825    -1.087178      23.00
 C      -3.917841     1.915647    -3.116985      13.95
 O      -3.748287     3.340984    -2.877449      83.93
 C      -3.112197     3.625514    -1.527140      98.71
 H      -2.620971     4.638292    -1.874987      22.73
 H      -2.357553     2.693218    -1.149655      22.41
 H      -3.923614     4.185628    -0.817949      23.56
 C      -3.562445     1.478536    -4.480588       2.44
 O      -3.243607     2.358254    -5.407187      52.31
 H      -3.373877     3.358105    -5.225728      17.95
 C      -3.560646     0.065093    -4.819218      52.41
 H      -3.311481    -0.343234    -5.852581      19.00
 C      -4.115197    -0.495065    -2.337497      12.13
 C      -4.467014    -1.416880    -1.168998     104.58
 H      -4.887205    -2.292885    -1.644571      26.04
 O      -5.524229    -1.296630    -0.123818      99.69
 H      -4.959332    -0.907984     0.748298      24.59
 C      -3.153830    -2.230003    -0.601230      68.66
 H      -2.432560    -2.468629    -1.364821      23.72
 C      -3.549024    -3.513760     0.059554      88.95
 O      -4.014861    -4.564111    -0.857052     233.57
 H      -3.637708    -4.291961    -1.784942      27.94
 H      -4.398814    -3.507338     0.773336      23.33
 H      -2.396004    -3.990563     0.459812      21.55
 C       1.131490    -1.785187    -0.012755      37.96
 H       1.849476    -2.673540    -0.162909      20.07
 C       0.769698     0.510090     0.693562      53.87
 H       1.338416     1.515210     1.050073      12.64
 C      -0.650805     0.293482     0.613621       8.88
 O      -1.564684     1.349961     0.797215     205.02
 C      -1.338656     2.360572     1.874463     108.47
 H      -0.458871     3.125700     1.564665      22.56
 H      -2.165180     3.262301     1.753867      22.84
 H      -1.534890     2.133023     3.049511      24.68
 C      -1.133983    -1.010082     0.076795      22.43
 O      -2.441065    -1.403870     0.484927     176.71
 C      -0.225144    -2.066796    -0.290751      41.88
 H      -0.813522    -2.759405    -0.855741      15.58
 C       1.645092    -0.565530     0.480382      56.84
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 C       3.133766    -0.337840     0.472368      69.60
 H       3.477920    -0.356869    -0.780517      16.80
 O       3.514289     1.051329     0.610668     282.72
 H       3.463194     1.469568     1.507090      27.99
 C       4.040860    -1.312283     1.128879      66.99
 H       4.203923    -0.640215     2.216647      19.74
 O       3.832388    -2.688623     1.062891     313.38
 H       3.679771    -3.138246     1.796490      31.57
 C       5.550881    -1.021027     0.683788      86.02
 O       6.228392     0.124727     1.278667     248.58
 H       5.661024     0.376821     1.973404      36.42
 H       5.992480    -1.046115    -0.356976      25.38
 H       6.063076    -2.003559     1.033518      27.90
55
name= lig-ACN-Water-frame_982
 C      -4.059459    -0.766439    -3.651015      57.84
 H      -4.321199    -1.811186    -3.822532      22.26
 C      -3.875321     0.965751    -1.985807      66.55
 H      -3.847266     1.331366    -1.057455      22.85
 C      -3.936897     1.890191    -3.059563      -0.37
 O      -3.732801     3.270129    -2.863884     158.29
 C      -3.072628     3.690117    -1.614467      85.73
 H      -2.135007     4.421426    -1.600368      22.54
 H      -2.429417     2.667554    -1.392638      22.99
 H      -3.792449     3.533957    -0.630143      22.08
 C      -3.592321     1.406497    -4.430303      15.57
 O      -3.176743     2.291830    -5.500121     119.11
 H      -3.395032     3.143305    -5.075750      23.10
 C      -3.523229     0.086386    -4.675693      49.09
 H      -3.359368    -0.218020    -5.805695      20.83
 C      -4.159134    -0.382071    -2.337891      27.96
 C      -4.482606    -1.620820    -1.371209      57.41
 H      -4.968349    -2.411428    -1.986657      24.89
 O      -5.583187    -1.253014    -0.239443     113.22
 H      -5.155136    -0.553655     0.424796      25.17
 C      -3.112423    -2.172883    -0.618299      67.01
 H      -2.471986    -2.169440    -1.462779      23.55
 C      -3.515106    -3.570271     0.025618      90.63
 O      -4.042062    -4.490113    -0.854219     251.93
 H      -3.301418    -4.682673    -1.733581      21.63
 H      -4.204106    -3.207168     0.855964      23.42
 H      -2.565017    -3.934443     0.875005      21.64
 C       1.231227    -1.774691    -0.180692      50.28
 H       1.936694    -2.376961    -0.805368      15.61
 C       0.602982     0.425006     0.718255     105.90
 H       0.765935     1.506537     1.221350      13.33
 C      -0.768279     0.283524     0.540726      18.17
 O      -1.670317     1.407867     0.805479     232.19
 C      -1.379793     2.383171     1.827760      87.64
 H      -0.224831     2.739906     1.858467      21.14
 H      -2.279885     3.097025     1.524559      21.18
 H      -1.455850     1.762389     2.892459      22.62
 C      -1.192739    -1.024007     0.221719      26.83
 O      -2.504714    -1.374983     0.430650     198.13
 C      -0.191386    -1.942495    -0.258712      48.28
 H      -0.231711    -2.879597    -0.636929      21.28
 C       1.663140    -0.610558     0.502430      70.56
 C       3.173874    -0.339338     0.381869      47.05
 H       3.450664    -0.671151    -0.829591      16.26
 O       3.648757     1.059656     0.637328     280.08
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 H       3.260383     1.229834     1.540034      23.87
 C       4.174360    -1.378378     1.195316      48.34
 H       4.015517    -1.336555     2.539625      18.18
 O       3.731811    -2.794068     1.057567     270.89
 H       3.604204    -3.150911     1.985762      25.82
 C       5.626739    -1.123292     0.589917      85.32
 O       6.143616     0.101335     1.316459     215.26
 H       5.584588     0.323874     2.097764      33.78
 H       5.327483    -0.793661    -0.383180      29.17
 H       6.361328    -2.027667     0.705731      27.03
55
name= lig-ACN-Water-frame_983
 C      -4.082009    -0.835078    -3.609089      50.55
 H      -4.246682    -1.868971    -3.992075      24.40
 C      -3.997400     1.010691    -1.901174      88.38
 H      -4.144510     1.357431    -0.933999      25.61
 C      -3.715323     1.879337    -3.042739       1.49
 O      -3.700566     3.236241    -2.805339     128.41
 C      -2.947498     3.551091    -1.629993     107.35
 H      -2.828233     4.733170    -1.973830      21.95
 H      -2.049990     2.885746    -1.251058      25.36
 H      -3.814746     3.935704    -0.810786      22.79
 C      -3.572750     1.484200    -4.376957      33.58
 O      -3.160604     2.236551    -5.457318      83.57
 H      -3.653959     3.034599    -5.649100      25.13
 C      -3.639581     0.029947    -4.548261      48.30
 H      -3.257840    -0.464766    -5.547616      19.91
 C      -4.228694    -0.369566    -2.241664     -20.28
 C      -4.464841    -1.584318    -1.343209      88.41
 H      -4.855664    -2.453602    -1.973157      24.56
 O      -5.519257    -1.201532    -0.464224     207.16
 H      -5.292776    -0.392980    -0.200305      33.82
 C      -3.200954    -2.187301    -0.724973      82.91
 H      -2.411986    -2.434577    -1.408566      25.53
 C      -3.439254    -3.486200     0.075507      84.72
 O      -4.083626    -4.479676    -0.867025     160.16
 H      -3.217227    -4.822124    -1.537939      23.84
 H      -4.313171    -3.422139     0.786005      23.49
 H      -2.370676    -4.139322     0.472840      21.97
 C       1.204721    -1.654478    -0.322213      41.69
 H       1.808684    -2.386865    -0.810127      22.56
 C       0.594007     0.384635     0.833626      82.58
 H       1.205020     1.365724     1.069013      18.98
 C      -0.824351     0.286326     0.570373      17.25
 O      -1.728518     1.309311     0.713043     181.61
 C      -1.428012     2.345865     1.820294      88.35
 H      -0.289629     2.670163     1.706808      22.09
 H      -1.852155     3.399442     1.975514      25.58
 H      -1.736948     1.758036     2.828415      25.01
 C      -1.186118    -1.056050     0.330047       4.67
 O      -2.656039    -1.298398     0.328235     139.75
 C      -0.172088    -1.938359    -0.224889      68.18
 H      -0.665838    -2.750690    -0.376107      24.10
 C       1.596367    -0.519422     0.388464      21.33
 C       3.307775    -0.334664     0.392384      49.45
 H       3.502937    -0.433801    -0.851056      19.48
 O       3.692271     0.963483     0.627942     276.83
 H       3.758831     1.180320     1.623250      23.37
 C       4.247642    -1.498231     1.243253      29.21
 H       4.374883    -1.071152     2.574143      22.57
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 O       3.668166    -2.850188     0.987337     246.43
 H       3.379825    -3.449610     1.919653      22.34
 C       5.579772    -1.096719     0.631777     112.56
 O       6.141906     0.010088     1.299823     185.48
 H       5.537843     0.207687     2.125350      34.49
 H       5.528964    -0.865172    -0.361366      29.74
 H       6.461290    -1.864740     0.460712      27.69
55
name= lig-ACN-Water-frame_984
 C      -4.063844    -0.851064    -3.536571      61.58
 H      -4.019929    -1.967286    -3.608397      25.46
 C      -4.153936     0.934746    -2.002735      67.64
 H      -4.293107     1.413471    -1.012630      30.53
 C      -3.588560     1.814201    -2.944094     -71.01
 O      -3.625292     3.204473    -2.758403     102.25
 C      -2.904248     3.722528    -1.586214      95.81
 H      -2.322243     4.784288    -1.828423      22.71
 H      -1.950294     3.072882    -1.577983      28.08
 H      -3.435094     3.508975    -0.460479      19.48
 C      -3.499535     1.362901    -4.312463      13.10
 O      -3.148652     2.211279    -5.420872     144.69
 H      -3.905418     2.892627    -5.455141      29.01
 C      -3.736052     0.063797    -4.597644      60.12
 H      -3.537655    -0.287168    -5.655091      20.90
 C      -4.211684    -0.433028    -2.267317      32.13
 C      -4.420594    -1.511595    -1.323196      92.49
 H      -4.845376    -2.352050    -1.987827      25.09
 O      -5.544003    -1.169654    -0.567851     146.75
 H      -5.551556    -0.255429    -0.110702      25.53
 C      -3.226674    -2.215498    -0.690848      76.58
 H      -2.610117    -2.323050    -1.613959      26.58
 C      -3.507686    -3.543698    -0.005037     108.63
 O      -4.099678    -4.495681    -0.817019     281.79
 H      -3.556629    -4.545310    -1.699103      27.32
 H      -3.876012    -3.385544     1.044139      25.13
 H      -2.235013    -3.647723     0.360647      22.65
 C       1.062890    -1.613996    -0.360556      27.09
 H       1.780366    -2.323847    -0.632304      23.94
 C       0.719184     0.501816     0.882818      49.65
 H       0.996552     1.481296     1.394371      18.50
 C      -0.701011     0.261427     0.736471      -7.08
 O      -1.783690     1.285424     0.664219     148.97
 C      -1.421102     2.245899     1.818060     101.45
 H      -0.304133     2.426197     1.805901      24.35
 H      -2.086753     2.904362     1.293540      24.75
 H      -1.688034     1.890174     2.941708      25.90
 C      -1.283700    -1.043472     0.292415       8.87
 O      -2.654334    -1.167925     0.214197     105.20
 C      -0.384461    -2.020860    -0.165084      80.20
 H      -0.468090    -2.838749    -0.659078      25.16
 C       1.722382    -0.465712     0.242664      23.78
 C       3.189486    -0.433535     0.467589      76.64
 H       3.683260    -0.814804    -0.607719      20.66
 O       3.735133     0.944913     0.652035     238.07
 H       3.921620     1.096793     1.643455      23.45
 C       4.114848    -1.535885     1.132664      52.69
 H       4.134288    -1.418138     2.538627      22.84
 O       3.685165    -2.820344     0.908335     255.02
 H       3.546875    -3.361176     1.868372      22.63
 C       5.632316    -1.186505     0.606128      89.05
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 O       6.227985    -0.025879     1.320355     242.03
 H       5.851447     0.190630     2.144006      36.12
 H       5.573754    -0.910071    -0.335154      32.55
 H       6.125425    -2.159561     0.981970      28.62
55
name= lig-ACN-Water-frame_985
 C      -3.940974    -0.913285    -3.682440      50.28
 H      -4.047345    -1.978011    -4.015365      23.29
 C      -4.204648     0.926857    -2.011596      60.65
 H      -4.627919     1.220312    -0.937320      22.40
 C      -3.625920     1.801166    -2.963199     -25.89
 O      -3.544842     3.239908    -2.709462     112.37
 C      -2.716302     3.802606    -1.557320      88.55
 H      -2.748854     5.034003    -1.595616      22.89
 H      -1.732469     3.271740    -1.476159      26.20
 H      -3.409315     3.615447    -0.548557      19.68
 C      -3.396595     1.320456    -4.289553       0.96
 O      -3.161294     2.184086    -5.338667     149.58
 H      -3.634976     3.098470    -5.310709      23.28
 C      -3.801032    -0.021176    -4.699954      43.18
 H      -4.032371    -0.212350    -5.706659      22.56
 C      -4.124011    -0.439348    -2.340071      25.03
 C      -4.529083    -1.576064    -1.350737      84.06
 H      -4.943203    -2.470690    -1.923018      23.83
 O      -5.738259    -1.140654    -0.472430     124.11
 H      -5.191143    -0.423517     0.227389      24.16
 C      -3.239700    -2.064551    -0.656760      86.88
 H      -2.456888    -2.316390    -1.439726      22.69
 C      -3.405569    -3.526897     0.044723      89.74
 O      -4.139746    -4.537398    -0.789905     279.82
 H      -3.753460    -4.567904    -1.579599      33.33
 H      -4.197646    -3.460296     0.816715      23.58
 H      -2.442500    -4.335972     0.273685      21.33
 C       0.925234    -1.644895    -0.226261      55.13
 H       1.433825    -2.338592    -0.833304      22.97
 C       0.797214     0.536556     0.841794      60.46
 H       1.208886     1.381649     1.343302      18.20
 C      -0.671756     0.170507     0.755836      20.35
 O      -1.615874     1.179778     0.794626     203.39
 C      -1.526167     2.220988     1.697719     135.59
 H      -0.529639     2.662788     1.792618      26.76
 H      -2.005977     3.165679     1.710346      26.41
 H      -1.999611     1.728268     2.680894      25.47
 C      -1.237198    -0.983902     0.224823      13.59
 O      -2.642252    -1.051970     0.128423     191.63
 C      -0.348462    -2.011399    -0.228259      43.58
 H      -0.810655    -2.849756    -0.548329      18.95
 C       1.550454    -0.453042     0.306448      43.76
 C       3.150739    -0.461248     0.339073      74.89
 H       3.324214    -0.571550    -0.837598      19.44
 O       3.729389     0.879388     0.668024     269.01
 H       3.585898     1.072181     1.649014      23.12
 C       4.035703    -1.415565     1.133930      74.91
 H       3.871480    -1.222199     2.470463      20.42
 O       3.706456    -2.855289     0.794426     274.47
 H       3.645305    -3.328801     1.600354      29.44
 C       5.592417    -1.297405     0.773901      97.18
 O       6.364030    -0.098006     1.293877     231.40
 H       6.115148    -0.009116     2.241905      34.53
 H       5.800845    -1.320128    -0.229311      30.48
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 H       6.223404    -2.226813     0.968385      28.54
55
name= lig-ACN-Water-frame_986
 C      -3.871940    -1.014117    -3.783352      43.48
 H      -4.230847    -2.032653    -4.014919      22.37
 C      -4.139296     0.864062    -2.033983      41.21
 H      -4.698740     1.327936    -1.044115      18.86
 C      -3.680365     1.874877    -2.944125      -2.92
 O      -3.432843     3.253714    -2.708433     171.29
 C      -2.667609     3.787768    -1.529548     106.65
 H      -2.777226     4.861604    -1.980960      23.74
 H      -1.583176     3.721656    -1.389144      25.89
 H      -3.204441     3.585014    -0.485938      22.39
 C      -3.451808     1.338313    -4.322193       5.96
 O      -3.126916     2.217242    -5.328908     200.35
 H      -3.412860     3.086618    -4.998152      23.28
 C      -3.753329     0.035608    -4.779551      46.67
 H      -3.833604    -0.167259    -5.769292      23.44
 C      -4.182074    -0.585098    -2.409513      -1.21
 C      -4.744187    -1.545888    -1.346861      75.14
 H      -5.137450    -2.499062    -1.770008      23.61
 O      -5.780174    -1.127155    -0.373419     186.97
 H      -5.312400    -0.715707     0.433845      25.92
 C      -3.207860    -2.125379    -0.646213      42.73
 H      -2.679764    -2.192344    -1.669957      21.81
 C      -3.434169    -3.541674     0.099156      93.07
 O      -4.191085    -4.514926    -0.795667     289.43
 H      -3.448412    -4.894195    -1.284487      29.23
 H      -3.951783    -3.390220     1.041811      25.32
 H      -2.253398    -3.653829     0.622836      20.98
 C       1.064776    -1.778158    -0.186624      41.45
 H       1.910657    -2.388037    -0.544027      19.98
 C       0.696404     0.464033     0.837168      72.25
 H       1.122863     1.398356     1.002950      20.86
 C      -0.606814     0.273818     0.727664      28.25
 O      -1.568665     1.145862     0.867242     213.78
 C      -1.584249     2.296835     1.800932     132.24
 H      -0.588790     2.687032     1.913994      25.32
 H      -2.276017     2.730088     1.192887      25.12
 H      -1.924600     1.983290     2.907622      26.07
 C      -1.207282    -0.972255     0.188559      13.44
 O      -2.632139    -0.923284     0.117063     163.71
 C      -0.456349    -1.960972    -0.288752      89.39
 H      -0.743179    -2.996636    -0.603371      22.09
 C       1.540974    -0.623795     0.416790      37.55
 C       3.110052    -0.339084     0.140384      80.68
 H       3.567025    -0.481646    -0.910189      23.66
 O       3.637481     0.831627     0.623203     221.70
 H       3.761778     0.799083     1.620530      25.61
 C       4.032187    -1.458790     1.090732      62.29
 H       3.647668    -1.050949     2.287865      23.21
 O       3.730420    -2.818484     0.706200     271.99
 H       3.556852    -3.350345     1.424398      31.88
 C       5.590047    -1.328563     0.965116     102.79
 O       6.459152    -0.257251     1.249192     202.08
 H       6.346790     0.158575     2.220511      29.74
 H       5.651319    -1.448693    -0.102508      28.84
 H       5.786685    -2.194220     1.635340      30.00
55
name= lig-ACN-Water-frame_987
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 C      -3.995019    -0.971920    -3.766453      56.35
 H      -3.907811    -2.004841    -4.125081      22.99
 C      -4.081175     0.730670    -2.124636      62.67
 H      -4.241747     0.944651    -0.969980      21.82
 C      -3.648363     1.756247    -2.990067      -2.99
 O      -3.324409     3.189078    -2.724129     206.26
 C      -2.705134     3.825791    -1.566501     123.68
 H      -2.678191     4.912939    -1.437452      26.71
 H      -1.819851     3.240482    -1.586139      26.31
 H      -3.224571     3.479175    -0.592045      25.58
 C      -3.566536     1.429605    -4.336492      25.17
 O      -3.077541     2.315839    -5.352926       4.15
 H      -3.489593     3.206287    -5.284139      16.90
 C      -3.622447     0.033364    -4.703995      48.63
 H      -3.246877    -0.116606    -5.660655      20.69
 C      -4.359109    -0.541115    -2.474636      26.18
 C      -4.732873    -1.593320    -1.256537      93.98
 H      -5.289180    -2.351978    -1.800617      23.85
 O      -5.737151    -1.129079    -0.315014     235.11
 H      -5.342319    -0.423712     0.146074      28.95
 C      -3.420658    -2.131222    -0.695001      68.08
 H      -2.644054    -2.450633    -1.501164      22.66
 C      -3.498771    -3.404932     0.140544     109.01
 O      -4.107803    -4.425552    -0.690161     196.36
 H      -3.338437    -4.969626    -1.328391      25.40
 H      -4.137472    -3.299579     0.982540      25.18
 H      -2.447342    -4.113776     0.242741      20.23
 C       1.070278    -1.925976    -0.151223      21.60
 H       1.529036    -2.941061    -0.384966      19.15
 C       0.809624     0.368191     0.813282      61.93
 H       1.148861     1.365638     1.071967      18.33
 C      -0.669171     0.210362     0.660623      11.78
 O      -1.706396     1.272511     0.995659     188.24
 C      -1.580326     2.354966     1.884541     137.15
 H      -0.888094     3.108502     1.794769      27.04
 H      -2.315068     3.114360     1.583633      26.57
 H      -2.154835     2.224476     2.862766      25.80
 C      -1.259252    -0.931334     0.159358      14.50
 O      -2.630964    -0.960966     0.080849     135.65
 C      -0.248972    -2.018003    -0.327595      48.76
 H      -0.771063    -2.874160    -0.977167      19.29
 C       1.716788    -0.703136     0.379808      42.15
 C       3.155538    -0.475636     0.170485      92.27
 H       3.153050    -0.500748    -0.926850      24.04
 O       3.550920     0.942737     0.565093     253.18
 H       3.543604     0.973724     1.584350      27.93
 C       3.928944    -1.393027     0.954826      89.13
 H       3.482444    -1.481860     2.117619      22.34
 O       3.758746    -2.780326     0.639363     211.18
 H       3.478473    -3.251359     1.581635      25.05
 C       5.549450    -1.468174     1.094634      97.41
 O       6.544650    -0.327552     1.245217     220.25
 H       6.313476     0.172158     2.055462      31.83
 H       6.040655    -2.071412     0.296173      29.28
 H       5.823876    -2.157273     1.873961      30.74
55
name= lig-ACN-Water-frame_988
 C      -4.123129    -0.893078    -3.813673      58.26
 H      -3.943616    -1.947658    -4.031374      23.39
 C      -4.050342     0.784318    -2.055304      51.11
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 H      -3.810198     1.063983    -1.006802      23.70
 C      -3.581664     1.789041    -3.014957     -18.66
 O      -3.310623     3.108604    -2.800576     191.52
 C      -2.745398     3.608986    -1.511588     127.75
 H      -2.728220     4.588964    -1.917438      26.44
 H      -1.727519     3.473967    -1.149351      27.48
 H      -3.466888     3.452287    -0.707983      26.15
 C      -3.547399     1.464224    -4.458589      18.70
 O      -3.090570     2.373004    -5.356406     110.72
 H      -3.620797     3.208717    -5.095861      22.55
 C      -3.485311     0.078063    -4.635005      50.66
 H      -3.044525    -0.441232    -5.489953      21.51
 C      -4.509963    -0.623284    -2.436539      -3.87
 C      -4.745698    -1.578266    -1.343565     103.53
 H      -5.073792    -2.554828    -1.650838      26.72
 O      -5.656153    -1.129245    -0.293943     229.10
 H      -5.466203    -0.321348     0.213766      24.73
 C      -3.421571    -2.092873    -0.692257      72.75
 H      -2.914461    -2.351029    -1.734771      26.49
 C      -3.563935    -3.346895     0.180401     101.62
 O      -4.084378    -4.401047    -0.607704     204.20
 H      -3.381220    -4.460827    -1.514851      23.25
 H      -4.164006    -3.247995     1.058577      25.98
 H      -2.373036    -3.218348     0.791284      22.81
 C       1.121861    -1.984780    -0.063428      36.67
 H       1.852567    -2.777278    -0.486304      16.05
 C       0.770170     0.251441     0.719025      64.34
 H       1.392414     1.027805     1.260950      19.00
 C      -0.653364     0.234692     0.711512      -9.24
 O      -1.773387     1.303615     1.058665      97.23
 C      -1.637927     2.550777     1.987535     118.82
 H      -0.660308     2.702026     1.914354      27.29
 H      -2.426468     3.173924     1.707632      26.91
 H      -1.469816     2.061381     2.925597      26.75
 C      -1.192711    -1.028041     0.031786      19.75
 O      -2.700484    -1.099786    -0.004843     114.53
 C      -0.344333    -1.958157    -0.327706      63.91
 H      -0.685332    -2.985328    -0.899653      23.00
 C       1.616688    -0.780623     0.306733      32.76
 C       3.205508    -0.390111     0.165211      77.14
 H       3.668994    -0.488581    -0.778546      21.37
 O       3.465294     0.986192     0.485014     314.50
 H       3.288430     1.229940     1.437244      26.66
 C       4.094173    -1.477131     1.029653      66.80
 H       3.761951    -0.903602     2.054131      22.78
 O       3.734888    -2.839284     0.551030     226.87
 H       3.441187    -3.486847     1.423696      25.24
 C       5.627627    -1.561948     1.227856     100.44
 O       6.545597    -0.392027     1.233860     264.78
 H       6.392498     0.105983     2.012925      34.62
 H       5.944240    -2.291296     0.378105      29.09
 H       5.510901    -1.913433     2.191729      30.96
55
name= lig-ACN-Water-frame_989
 C      -4.182760    -0.844293    -3.746435      46.01
 H      -4.510611    -1.795372    -4.174061      24.47
 C      -4.032836     0.854876    -2.047137      96.73
 H      -4.013856     1.183989    -1.079570      25.15
 C      -3.648996     1.704952    -3.058271      24.21
 O      -3.238757     3.015304    -2.804878     209.08
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 C      -2.855801     3.499217    -1.506434     131.21
 H      -2.681547     4.540921    -1.520256      28.58
 H      -1.984720     2.854759    -1.275069      28.20
 H      -3.607997     3.413324    -0.767335      28.01
 C      -3.405373     1.384309    -4.396419       9.05
 O      -3.140531     2.392687    -5.393563      66.60
 H      -3.428029     3.330140    -5.128199      22.46
 C      -3.453029    -0.002336    -4.703615      35.20
 H      -3.132816    -0.200776    -5.805052      18.88
 C      -4.448269    -0.400990    -2.453792      35.98
 C      -4.789350    -1.579246    -1.354590      85.94
 H      -5.349792    -2.334736    -1.842165      25.78
 O      -5.682559    -1.187928    -0.325494     219.30
 H      -5.073553    -0.574219     0.299725      24.05
 C      -3.338657    -2.122248    -0.794993      77.99
 H      -2.602843    -2.576055    -1.576177      24.97
 C      -3.625432    -3.214144     0.257411      89.71
 O      -4.020444    -4.425957    -0.533419     236.52
 H      -3.437488    -4.503013    -1.322741      29.34
 H      -4.481641    -2.920744     0.857508      26.47
 H      -2.537885    -3.712571     0.864526      21.88
 C       1.026590    -2.020143    -0.156051      36.60
 H       1.730207    -2.833652    -0.527578      19.26
 C       0.656488     0.281300     0.745130      55.30
 H       0.988781     1.359138     1.146865      20.83
 C      -0.785407     0.263327     0.711144      18.32
 O      -1.728845     1.221116     1.068650     158.03
 C      -1.462063     2.483840     2.061768     123.01
 H      -0.852889     3.189894     1.757758      29.46
 H      -2.279609     3.095738     1.841551      29.00
 H      -1.720751     2.362647     3.053129      29.11
 C      -1.310698    -0.908171     0.047450      13.36
 O      -2.632231    -1.097326    -0.041519     133.37
 C      -0.349262    -2.109318    -0.346656      50.37
 H      -0.928250    -3.111309    -0.656106      22.07
 C       1.642970    -0.739706     0.248950      22.82
 C       3.287245    -0.371397     0.120800      70.54
 H       3.421881    -0.481361    -0.881664      25.23
 O       3.393508     1.010816     0.443760     300.93
 H       3.536648     0.994856     1.435130      27.77
 C       4.163142    -1.480232     1.152402      80.71
 H       3.665414    -1.933523     2.130240      22.95
 O       3.710294    -2.843961     0.553285     209.20
 H       3.563701    -3.401860     1.319270      29.92
 C       5.746936    -1.613517     1.373758     101.51
 O       6.507541    -0.458876     1.213388     217.83
 H       6.434527     0.109727     2.081238      28.51
 H       6.273130    -2.344191     0.572259      29.46
 H       6.080763    -2.135519     2.203845      31.99
55
name= lig-ACN-Water-frame_990
 C      -4.155342    -0.797568    -3.800944      42.44
 H      -4.711969    -1.727392    -3.975497      23.16
 C      -4.058229     0.974779    -2.003665      55.21
 H      -4.371684     1.241577    -1.071396      20.64
 C      -3.599907     1.777167    -3.059140       3.14
 O      -3.185208     3.065477    -2.846045     187.93
 C      -2.957453     3.337866    -1.425334     121.00
 H      -2.443245     4.214786    -1.401549      28.48
 H      -2.294453     2.625108    -0.891147      27.29
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 H      -3.850059     3.252586    -0.932879      27.66
 C      -3.282250     1.296099    -4.430364      10.59
 O      -3.146467     2.251771    -5.391042      46.76
 H      -3.792167     2.988027    -5.130163      19.78
 C      -3.568793    -0.027583    -4.788462      56.37
 H      -3.648526    -0.512586    -5.877293      20.57
 C      -4.375045    -0.431319    -2.415914       3.06
 C      -4.704651    -1.495468    -1.474920      81.11
 H      -5.126140    -2.258600    -2.081047      27.04
 O      -5.710208    -1.262959    -0.343978     155.83
 H      -5.402077    -0.508061     0.430890      20.65
 C      -3.333721    -2.195103    -0.836234      69.29
 H      -2.663475    -2.471042    -1.697798      25.93
 C      -3.680054    -3.248087     0.170196      97.44
 O      -4.004956    -4.456998    -0.431665     306.79
 H      -3.267316    -4.731110    -0.824396      33.69
 H      -4.520923    -2.905945     0.820614      24.32
 H      -2.710599    -3.261714     1.201429      21.78
 C       0.940003    -1.911990    -0.315898      41.45
 H       1.409655    -2.880096    -0.418343      22.60
 C       0.632391     0.347906     0.752147      49.81
 H       1.181155     1.437369     0.956353      17.15
 C      -0.776013     0.188114     0.644977      12.67
 O      -1.635934     1.211684     1.161502     186.64
 C      -1.391318     2.358884     1.978851     135.66
 H      -0.524441     2.790163     1.805848      27.26
 H      -2.342889     2.777006     1.860505      25.75
 H      -1.125326     1.904232     2.867443      27.77
 C      -1.256066    -1.049198     0.045101      23.16
 O      -2.683175    -0.965686    -0.061240     140.90
 C      -0.469008    -2.043976    -0.247449      69.92
 H      -0.863557    -3.044043    -0.536226      20.43
 C       1.573240    -0.647779     0.270954      26.38
 C       3.206213    -0.492289     0.231120      77.42
 H       3.646725    -0.689692    -0.643908      24.66
 O       3.401044     1.003197     0.477496     263.23
 H       3.686298     1.165156     1.402701      26.46
 C       4.084187    -1.627092     1.199200      76.86
 H       3.682755    -1.005106     2.218869      20.48
 O       3.747986    -2.812724     0.567323     299.64
 H       3.616179    -3.447663     1.181447      31.62
 C       5.824374    -1.708664     1.417775      74.98
 O       6.531787    -0.392429     1.243338     229.65
 H       6.352485     0.160399     2.130769      26.88
 H       5.992338    -2.318122     0.389950      28.37
 H       5.902451    -2.086427     2.350393      30.96
55
name= lig-ACN-Water-frame_991
 C      -4.186790    -0.869943    -3.741275      52.27
 H      -4.210191    -1.916742    -4.062057      24.84
 C      -4.123213     0.953869    -2.102570      72.29
 H      -4.291522     1.389043    -1.117141      24.82
 C      -3.448115     1.772465    -3.093711     -25.98
 O      -3.137820     3.162195    -2.855927     149.59
 C      -3.038752     3.248511    -1.301110     111.44
 H      -2.509780     4.116346    -1.198593      28.74
 H      -2.569076     2.368607    -0.840253      28.18
 H      -3.894141     3.575265    -0.933068      27.93
 C      -3.342774     1.242115    -4.402726      11.16
 O      -3.112488     2.137387    -5.442374     127.49
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 H      -3.617352     3.011645    -5.418527      21.77
 C      -3.759903    -0.029658    -4.809173      37.71
 H      -3.752894    -0.281019    -5.976051      18.61
 C      -4.273754    -0.355719    -2.452549      12.47
 C      -4.641448    -1.545144    -1.422903      74.35
 H      -5.039687    -2.395485    -1.945656      23.13
 O      -5.697579    -1.320255    -0.446955     187.88
 H      -5.236240    -0.665996     0.216673      25.87
 C      -3.402615    -2.010247    -0.822572      99.35
 H      -2.770689    -2.426888    -1.606794      28.80
 C      -3.721738    -3.216903     0.184241      86.81
 O      -3.989512    -4.575072    -0.342738     196.76
 H      -3.141740    -5.096457    -0.717396      26.72
 H      -4.695685    -2.943715     0.694736      24.48
 H      -2.608086    -3.224485     1.006383      22.73
 C       0.927796    -1.751270    -0.296709      47.36
 H       1.683329    -2.347121    -0.701164      23.74
 C       0.760454     0.366410     0.665856      75.04
 H       1.179433     1.362344     1.285134      18.84
 C      -0.639374     0.204741     0.671732      17.25
 O      -1.647426     1.064034     1.103191     194.23
 C      -1.210458     2.167534     1.969095     142.41
 H      -0.598194     2.741461     1.451567      29.26
 H      -1.814483     2.948043     2.242571      29.01
 H      -0.936130     1.905457     2.928477      29.98
 C      -1.421673    -0.953394     0.149757       1.31
 O      -2.760227    -0.961991    -0.146433     163.24
 C      -0.482213    -2.073157    -0.250949      64.29
 H      -0.803178    -2.984668    -0.614719      22.00
 C       1.528292    -0.703772     0.238187      45.29
 C       3.110316    -0.518515     0.357171      89.71
 H       3.340666    -0.699993    -0.602308      24.96
 O       3.467676     0.896212     0.513614     297.35
 H       3.473994     1.016085     1.506771      25.29
 C       4.044133    -1.506869     1.235736      76.40
 H       3.689136    -1.876740     2.475089      20.30
 O       3.744877    -2.851248     0.633139     229.41
 H       3.542067    -3.549757     1.439849      25.06
 C       5.664649    -1.570596     1.320137      99.13
 O       6.528184    -0.380373     1.332546     259.19
 H       6.402663     0.059376     2.194263      30.33
 H       6.299858    -2.314422     0.623843      29.17
 H       5.859083    -2.065436     2.174975      32.18
55
name= lig-ACN-Water-frame_992
 C      -4.137068    -0.985308    -3.779293      79.39
 H      -4.214402    -2.065312    -3.807076      25.64
 C      -4.080573     0.968840    -2.248631      43.78
 H      -4.387302     1.218972    -1.147339      23.29
 C      -3.418106     1.785444    -3.113702       2.40
 O      -3.088656     3.107411    -2.750505     179.28
 C      -3.088605     3.381883    -1.275826     130.50
 H      -2.261642     3.856104    -0.884404      28.42
 H      -2.874606     2.407190    -0.913790      28.10
 H      -3.994389     3.477823    -0.964715      30.58
 C      -3.506252     1.347252    -4.467822      12.87
 O      -3.032659     2.077524    -5.560492     157.88
 H      -3.330079     2.992282    -5.392968      26.71
 C      -3.906174     0.002127    -4.738660      65.00
 H      -3.804629    -0.242911    -5.848144      22.82
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 C      -4.339966    -0.498004    -2.465134     -39.14
 C      -4.694429    -1.551406    -1.466213      95.88
 H      -5.022903    -2.387206    -2.116406      24.33
 O      -5.692097    -1.293925    -0.528126     231.21
 H      -5.482371    -0.717921     0.119346      29.73
 C      -3.354927    -2.091878    -0.763723      90.55
 H      -2.722433    -2.386307    -1.557599      30.40
 C      -3.716859    -3.226862     0.212434      87.83
 O      -3.961473    -4.647552    -0.262572     175.66
 H      -3.036470    -4.816334    -0.953816      24.06
 H      -4.589644    -3.018877     0.927874      23.87
 H      -2.730987    -3.424878     1.155267      22.54
 C       0.907315    -1.861739    -0.316152      63.62
 H       1.255489    -2.634747    -0.935487      22.61
 C       0.731271     0.416299     0.718417      65.84
 H       1.283709     1.323840     1.320197      19.11
 C      -0.743898     0.153073     0.653403      17.74
 O      -1.696994     1.045046     1.114664     175.21
 C      -0.990271     2.084060     1.973287     121.80
 H      -0.316743     2.572127     1.407445      28.67
 H      -1.948674     2.391018     2.161779      25.85
 H      -0.419055     1.635709     2.689617      29.78
 C      -1.284105    -1.017802     0.137886      21.12
 O      -2.774388    -0.865454    -0.113049     114.24
 C      -0.490553    -1.982432    -0.322073      48.13
 H      -0.882691    -2.772898    -0.759282      24.61
 C       1.633757    -0.605147     0.335569      47.71
 C       3.132193    -0.545925     0.354362      96.63
 H       3.516664    -0.820105    -0.545033      25.74
 O       3.548014     0.764812     0.587791     294.33
 H       3.443598     1.030745     1.562498      25.02
 C       3.962177    -1.526661     1.228231      53.43
 H       3.511268    -1.326783     2.537969      21.83
 O       3.728866    -2.899426     0.698871     226.13
 H       3.516368    -3.501861     1.676623      21.97
 C       5.536914    -1.404437     1.283571     100.77
 O       6.469053    -0.349804     1.432545     296.24
 H       6.423130     0.055949     2.288875      31.40
 H       5.614398    -1.820212     0.161593      28.60
 H       5.687811    -2.091921     2.019873      32.13
55
name= lig-ACN-Water-frame_993
 C      -4.110002    -0.993496    -3.813329      53.25
 H      -4.367761    -1.878062    -4.339840      18.43
 C      -4.086790     0.766837    -2.211554      54.38
 H      -4.334487     1.279754    -1.174565      21.39
 C      -3.565028     1.821903    -3.146694     -14.31
 O      -3.007493     3.061948    -2.675832     143.96
 C      -3.120158     3.377077    -1.249518     134.56
 H      -2.534870     4.265107    -1.367629      27.07
 H      -2.934435     2.679207    -0.504778      28.45
 H      -3.880774     3.963074    -1.079534      30.71
 C      -3.593691     1.418603    -4.572534      17.97
 O      -2.994793     2.063070    -5.649138     126.70
 H      -3.162012     3.027110    -5.667358      23.30
 C      -3.920433     0.026872    -4.783548      22.09
 H      -3.956229    -0.335118    -5.787754      25.43
 C      -4.385620    -0.527250    -2.540359      43.39
 C      -4.669104    -1.616676    -1.488038      80.72
 H      -5.167459    -2.523762    -1.923924      27.22
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 O      -5.804885    -1.237046    -0.550441     163.47
 H      -5.446746    -0.428917    -0.085401      27.25
 C      -3.360067    -2.183114    -0.729031      58.26
 H      -2.686180    -2.572608    -1.439335      28.98
 C      -3.650449    -3.360714     0.366289      93.38
 O      -3.894035    -4.595624    -0.239601     241.04
 H      -3.248907    -4.788854    -1.065072      27.13
 H      -4.632064    -2.994833     0.814216      24.97
 H      -2.548414    -3.151709     1.130882      24.85
 C       1.010464    -1.858257    -0.272927      24.12
 H       1.809218    -2.602581    -0.406794      17.29
 C       0.619316     0.290074     0.805864      90.64
 H       0.960520     1.344543     0.995226      18.18
 C      -0.726651     0.163004     0.668166      17.43
 O      -1.634521     1.112151     1.178113     231.01
 C      -0.945091     2.019957     1.973011     137.73
 H      -0.440190     2.760708     1.443794      28.70
 H      -1.211670     2.735789     2.677088      28.05
 H      -0.337227     1.491679     2.573666      30.56
 C      -1.337531    -0.956744     0.067292      20.64
 O      -2.672417    -0.902542    -0.027935     110.31
 C      -0.442985    -1.992690    -0.478430      76.26
 H      -0.737067    -2.861795    -0.978292      25.46
 C       1.494422    -0.777629     0.285715      43.21
 C       3.214970    -0.603930     0.246999      71.83
 H       3.513357    -0.716553    -0.726556      26.52
 O       3.669290     0.754156     0.644799     217.56
 H       3.619519     0.855128     1.644546      26.37
 C       3.811784    -1.540810     1.269689      71.35
 H       3.327039    -1.181011     2.516377      22.07
 O       3.705887    -2.855766     0.818545     224.62
 H       3.632156    -3.651347     1.618995      24.18
 C       5.417241    -1.412280     1.176525      92.62
 O       6.352949    -0.252767     1.513182     253.15
 H       6.337449     0.157506     2.412806      27.68
 H       5.760496    -1.470648     0.056404      27.82
 H       5.842490    -2.283444     1.469021      33.11
55
name= lig-ACN-Water-frame_994
 C      -4.206576    -0.907213    -3.994805      46.01
 H      -4.348458    -1.949512    -4.171870      26.63
 C      -4.084840     0.782661    -2.189774      39.15
 H      -4.036678     0.940362    -1.069411      19.07
 C      -3.759100     1.735326    -3.153637      20.12
 O      -2.995554     2.886941    -2.671639     211.47
 C      -3.147142     3.564965    -1.283684     117.55
 H      -2.263188     4.195547    -1.096619      25.04
 H      -2.853358     2.830372    -0.571033      25.69
 H      -4.120238     3.659501    -1.092910      26.62
 C      -3.578482     1.393273    -4.536695      24.05
 O      -3.009399     2.096573    -5.697884      50.58
 H      -3.334895     3.041887    -5.503430      25.60
 C      -3.847556     0.100814    -4.963997      63.15
 H      -3.771957    -0.075687    -5.966474      25.96
 C      -4.342196    -0.627674    -2.540761     -36.58
 C      -4.722149    -1.718108    -1.357329      80.81
 H      -5.017617    -2.636212    -1.971516      23.72
 O      -5.839991    -1.172562    -0.597805     189.84
 H      -5.478812    -0.366621     0.095706      21.02
 C      -3.404320    -2.165857    -0.627147      95.23
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 H      -2.802935    -2.549125    -1.444754      26.34
 C      -3.574553    -3.272355     0.426994     100.60
 O      -3.827622    -4.576076    -0.252167     285.01
 H      -3.087273    -4.766308    -0.717339      33.27
 H      -4.422602    -3.215426     1.170418      23.51
 H      -2.647123    -3.653256     1.285847      22.33
 C       0.994024    -1.978185    -0.275789      64.70
 H       1.620566    -2.907664    -0.578180      16.32
 C       0.684201     0.160855     0.782710      64.60
 H       1.262774     0.995415     1.091794      18.36
 C      -0.778767     0.142065     0.698915      12.42
 O      -1.622992     1.172399     1.229262     174.30
 C      -0.786746     2.139571     2.132303     106.09
 H      -0.407101     2.736658     1.352596      25.75
 H      -1.752788     2.333302     2.593976      23.85
 H      -0.001516     1.666863     2.562598      27.68
 C      -1.260050    -0.985474    -0.089566      28.31
 O      -2.694478    -1.119610    -0.016541     211.09
 C      -0.361938    -1.993418    -0.560159      57.00
 H      -0.831180    -2.925954    -1.014948      22.03
 C       1.582638    -0.718351     0.288894      43.78
 C       3.068037    -0.499793     0.261061      77.82
 H       3.418086    -0.779209    -0.707692      22.15
 O       3.738573     0.729130     0.612721     271.37
 H       3.412186     0.935538     1.535574      26.26
 C       3.894831    -1.491252     1.246851      56.40
 H       3.310810    -1.550626     2.477730      20.59
 O       3.623142    -2.869311     0.884464     262.79
 H       3.620987    -3.404816     1.730232      27.27
 C       5.449250    -1.366798     1.053838     101.98
 O       6.161541    -0.217945     1.515459     268.65
 H       6.192916    -0.049364     2.482982      27.26
 H       5.418696    -1.346267    -0.066903      30.78
 H       5.827517    -2.220885     1.512467      31.57
55
name= lig-ACN-Water-frame_995
 C      -4.329345    -0.893339    -4.006890      56.68
 H      -4.381357    -1.860507    -4.485775      25.26
 C      -4.124608     0.664731    -2.190257      53.44
 H      -3.879952     0.988269    -1.220703      19.47
 C      -3.722828     1.710700    -3.087082       9.24
 O      -3.002770     2.795905    -2.686310     204.50
 C      -3.189679     3.513575    -1.386288     108.84
 H      -2.698670     4.560327    -1.555844      23.73
 H      -2.794734     2.887125    -0.603885      23.30
 H      -4.096714     3.918777    -1.166555      25.73
 C      -3.515949     1.377480    -4.578449       4.27
 O      -3.094849     2.224851    -5.571092     117.45
 H      -3.238334     3.192185    -5.305816      25.89
 C      -3.842904     0.053277    -5.038091      44.07
 H      -3.605643    -0.193751    -6.031863      21.39
 C      -4.294674    -0.672759    -2.607938      24.30
 C      -4.728304    -1.653822    -1.393413      75.63
 H      -5.241688    -2.647685    -1.676168      23.13
 O      -5.829707    -1.135198    -0.620454     198.29
 H      -5.392711    -0.729733     0.259812      23.26
 C      -3.444725    -2.247981    -0.567496      78.34
 H      -2.929909    -2.730154    -1.405175      24.22
 C      -3.566594    -3.348146     0.489719      96.77
 O      -3.774334    -4.562083    -0.253165     281.08
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 H      -2.912900    -4.902855    -0.628931      27.46
 H      -4.335335    -3.041369     1.201783      24.58
 H      -2.382211    -3.047731     0.877315      19.83
 C       1.053561    -1.994077    -0.320175      52.03
 H       1.574061    -2.920215    -0.840765      15.93
 C       0.694141     0.234925     0.775540      62.56
 H       0.950852     0.931338     1.428500      18.65
 C      -0.703195     0.081067     0.640064      10.85
 O      -1.496405     1.107443     1.267658     134.63
 C      -0.778683     2.236802     2.192250     102.35
 H      -0.425614     3.239519     1.856878      24.43
 H      -1.476743     2.689701     2.960752      25.44
 H      -0.117367     1.854701     2.928189      26.67
 C      -1.267607    -1.002991    -0.114366      34.31
 O      -2.654262    -1.171190     0.009024     189.60
 C      -0.386798    -1.991963    -0.542813      62.92
 H      -0.844041    -3.007001    -1.068613      18.58
 C       1.586345    -0.844270     0.238043      57.99
 C       3.131994    -0.549617     0.380025      79.52
 H       3.415633    -0.692766    -0.684737      20.66
 O       3.657365     0.792554     0.534865     247.34
 H       3.586004     1.179782     1.440009      26.58
 C       3.910469    -1.505639     1.201414      55.60
 H       4.009657    -0.807618     2.311737      19.74
 O       3.534516    -2.856785     0.835616     301.97
 H       3.540145    -3.406225     1.586453      30.74
 C       5.417025    -1.363430     0.954316     113.32
 O       6.021538    -0.158743     1.447735     204.91
 H       6.024229    -0.159937     2.501491      28.31
 H       5.814251    -1.454160    -0.058723      30.99
 H       5.906975    -2.215909     1.398286      31.63
55
name= lig-ACN-Water-frame_996
 C      -4.333328    -0.993117    -4.049212      60.56
 H      -4.798737    -1.934102    -4.378416      27.08
 C      -4.051368     0.624962    -2.224488      72.72
 H      -4.264215     0.782873    -1.268269      24.70
 C      -3.559391     1.551805    -3.169760       5.84
 O      -3.013594     2.808693    -2.724159     207.52
 C      -3.261836     3.469478    -1.522704     119.71
 H      -2.589796     4.389781    -1.789025      24.20
 H      -2.721184     3.224733    -0.585757      26.45
 H      -4.292595     3.469198    -1.346606      27.07
 C      -3.551091     1.325779    -4.527099      15.68
 O      -3.146891     2.392246    -5.394304     -31.32
 H      -3.430933     3.257302    -4.906835      18.59
 C      -3.866336     0.022079    -4.903816      60.40
 H      -3.891462    -0.346900    -5.955103      21.85
 C      -4.393312    -0.681880    -2.635877      -0.83
 C      -4.696880    -1.669069    -1.491212      78.88
 H      -5.096563    -2.526298    -2.157673      23.88
 O      -5.792117    -1.096094    -0.575803     200.92
 H      -5.434079    -0.571722     0.082185      28.01
 C      -3.494169    -2.269768    -0.704238      68.68
 H      -2.706955    -2.669195    -1.401827      23.53
 C      -3.529495    -3.354411     0.473754     106.56
 O      -3.751525    -4.610662    -0.181956     184.72
 H      -2.868187    -4.893946    -0.868819      23.14
 H      -4.321551    -3.426824     1.177577      24.55
 H      -2.577522    -3.601274     1.230563      22.92
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 C       1.004813    -1.910057    -0.437196      37.63
 H       1.925324    -2.555120    -0.676589      18.76
 C       0.775344     0.152849     0.735685      70.76
 H       1.258417     0.913095     1.167430      22.73
 C      -0.611874     0.164037     0.616691      20.32
 O      -1.351781     1.106471     1.354212     192.88
 C      -0.864365     2.232595     2.268396      95.97
 H      -0.360349     2.777744     1.395062      23.62
 H      -1.869698     2.526444     2.710678      24.63
 H      -0.047763     1.762581     2.817620      25.64
 C      -1.266653    -1.001703     0.011198      27.11
 O      -2.642029    -1.064935     0.044592      77.98
 C      -0.394912    -2.045841    -0.507005      63.15
 H      -0.866054    -3.076516    -1.125524      17.70
 C       1.577242    -0.822935     0.316314      45.68
 C       3.188417    -0.558538     0.263864      66.15
 H       3.603488    -0.912182    -0.766939      23.59
 O       3.476057     0.904169     0.468979     241.87
 H       3.624888     0.889259     1.445863      24.91
 C       4.020650    -1.499425     1.186080      94.85
 H       3.613903    -1.800630     2.314113      20.41
 O       3.445197    -2.771890     0.799258     297.40
 H       3.481547    -3.429730     1.527121      30.88
 C       5.510794    -1.466406     0.840833      96.27
 O       5.954385    -0.071498     1.402467     186.27
 H       5.983543     0.079451     2.423395      27.09
 H       5.652737    -1.440035    -0.183808      32.08
 H       5.968079    -2.293068     1.412752      30.78
55
name= lig-ACN-Water-frame_997
 C      -4.339680    -1.077137    -3.953611      55.69
 H      -4.688909    -2.056440    -4.366300      20.54
 C      -3.971559     0.597551    -2.237829      83.82
 H      -4.079174     1.017509    -1.307847      25.46
 C      -3.393363     1.501569    -3.052111      -1.71
 O      -2.986385     2.757359    -2.881423     208.28
 C      -3.323279     3.484672    -1.575022     120.38
 H      -3.296353     4.657549    -1.543937      25.21
 H      -2.773726     2.811098    -0.910508      25.48
 H      -4.364242     3.455949    -1.337389      27.87
 C      -3.531145     1.304545    -4.508791      -6.24
 O      -3.187809     2.366263    -5.238526      86.41
 H      -3.613346     3.253727    -5.033546      21.08
 C      -3.936375    -0.037827    -4.940061      39.97
 H      -4.100731     0.003167    -6.103777      20.07
 C      -4.455900    -0.698173    -2.634412      52.91
 C      -4.756085    -1.687279    -1.532173      74.34
 H      -5.313242    -2.647757    -1.763689      24.90
 O      -5.704491    -1.141559    -0.586610     212.15
 H      -5.265270    -0.419816    -0.137625      27.62
 C      -3.318838    -2.158066    -0.693446      55.32
 H      -2.737650    -2.474830    -1.639438      27.41
 C      -3.586800    -3.405662     0.401106      98.88
 O      -3.749756    -4.747699    -0.151621     225.97
 H      -2.899948    -4.792838    -0.923697      24.05
 H      -4.383975    -2.971162     0.913625      26.87
 H      -2.579542    -3.065290     0.959015      26.29
 C       1.013486    -1.839891    -0.482737      10.96
 H       1.267019    -2.689749    -1.101527      22.04
 C       0.877221     0.231653     0.793457      52.80
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 H       1.326021     1.170260     0.995992      21.28
 C      -0.569273     0.190462     0.709092      14.69
 O      -1.370194     1.052217     1.406621     218.79
 C      -0.866988     2.080745     2.134300     139.99
 H      -0.508093     3.187286     1.779562      25.28
 H      -1.783653     2.566008     2.651110      25.95
 H      -0.356776     2.030483     3.125281      26.78
 C      -1.197907    -1.006202     0.132399       8.82
 O      -2.747202    -0.984464     0.025131      75.22
 C      -0.381771    -1.987148    -0.445062      57.72
 H      -0.945496    -3.040959    -1.000297      18.84
 C       1.736081    -0.843692     0.223846      39.88
 C       3.138132    -0.481106     0.175733      79.18
 H       3.520389    -0.598511    -0.961781      23.90
 O       3.288671     0.913661     0.411937     206.12
 H       3.628001     1.176142     1.315136      25.87
 C       4.015946    -1.592551     1.184716      59.12
 H       4.009217    -0.879735     2.257318      22.56
 O       3.378912    -2.794726     0.707906     236.08
 H       3.598730    -3.609142     1.430485      25.58
 C       5.586083    -1.401895     0.924323     113.24
 O       5.948961    -0.076435     1.311638     222.14
 H       5.867765    -0.073347     2.238602      33.06
 H       5.717644    -1.462374    -0.071690      32.98
 H       6.416030    -2.142558     1.225006      30.36
55
name= lig-ACN-Water-frame_998
 C      -4.331906    -1.000752    -4.025888      34.95
 H      -4.427261    -2.080166    -4.312491      23.76
 C      -3.946458     0.561305    -2.096573      14.25
 H      -3.864895     0.631880    -0.992693      24.90
 C      -3.346099     1.457732    -3.113779      -4.75
 O      -2.928542     2.895734    -2.888471     199.49
 C      -3.427115     3.354761    -1.636938     119.46
 H      -3.032036     4.437563    -1.887437      24.84
 H      -2.821440     3.278943    -0.665825      26.12
 H      -4.440191     3.040251    -1.496323      27.40
 C      -3.498703     1.129153    -4.426256      17.72
 O      -3.215507     2.241909    -5.285042     199.88
 H      -3.495444     2.977237    -4.741539      24.80
 C      -4.029462    -0.014720    -4.953582      79.10
 H      -4.152501    -0.374117    -6.075258      22.85
 C      -4.396962    -0.724097    -2.585391     -21.34
 C      -4.701295    -1.717303    -1.410526      95.21
 H      -4.979677    -2.678161    -1.870551      26.00
 O      -5.667421    -1.180215    -0.557155     194.49
 H      -5.275744    -0.450924     0.174652      20.40
 C      -3.297397    -2.091654    -0.740507      96.15
 H      -2.417968    -2.403523    -1.433426      26.03
 C      -3.573937    -3.263088     0.222028     112.66
 O      -3.742529    -4.788494    -0.120305     209.59
 H      -3.031740    -5.141520    -0.727124      28.37
 H      -4.509264    -3.264173     0.712982      26.95
 H      -2.870322    -3.549144     1.086163      25.21
 C       1.028770    -1.867715    -0.505215      24.01
 H       1.749657    -2.381911    -1.042728      18.71
 C       0.888584     0.236957     0.773497      69.46
 H       1.255717     1.168547     1.350918      22.04
 C      -0.482521     0.036798     0.857102      19.85
 O      -1.458965     0.957289     1.376671     101.10
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 C      -0.932639     2.180973     2.213092     101.32
 H      -0.172948     2.689129     1.340711      23.63
 H      -1.918581     2.613641     2.579686      24.19
 H      -0.249499     1.483122     2.758318      23.99
 C      -1.279187    -0.919500     0.222474      29.97
 O      -2.690111    -0.976793    -0.018257     146.47
 C      -0.417729    -1.862193    -0.355301      71.48
 H      -0.904949    -2.948324    -0.904529      20.34
 C       1.615635    -0.722427     0.080205      21.81
 C       3.246419    -0.497113     0.121716      72.92
 H       3.666691    -0.644318    -1.031928      23.04
 O       3.203741     0.979798     0.372740     209.55
 H       3.590202     1.092184     1.274999      26.75
 C       4.002300    -1.472886     1.019711      81.49
 H       3.497105    -1.493103     2.211502      21.83
 O       3.406156    -2.831733     0.723278     261.76
 H       3.677600    -3.487756     1.519153      29.19
 C       5.590441    -1.394281     0.869983     100.86
 O       5.984477    -0.057703     1.288636     180.19
 H       5.909819     0.213129     2.231332      28.33
 H       5.895283    -1.506054    -0.091422      32.66
 H       5.931811    -2.172162     1.679836      30.41
55
name= lig-ACN-Water-frame_999
 C      -4.376228    -1.021880    -3.912987      58.72
 H      -4.738341    -1.999404    -4.301071      20.90
 C      -3.837434     0.559734    -2.115795      70.24
 H      -3.709655     0.839090    -0.962429      20.71
 C      -3.390117     1.458211    -3.012484      -2.31
 O      -2.887838     2.774771    -2.848678     241.33
 C      -3.470020     3.403180    -1.662685     115.30
 H      -3.791662     4.524156    -1.662109      25.50
 H      -2.902127     2.882956    -0.810525      24.19
 H      -4.519780     3.058017    -1.598055      26.58
 C      -3.462817     1.158015    -4.499404      -8.20
 O      -3.244221     2.087720    -5.395980     155.50
 H      -3.135315     2.980037    -4.972165      22.07
 C      -4.070275    -0.082207    -4.935051      53.33
 H      -4.010950    -0.213389    -6.083746      22.74
 C      -4.254999    -0.696899    -2.561354      54.03
 C      -4.478927    -1.677343    -1.455761      78.10
 H      -4.956211    -2.567232    -1.788100      27.77
 O      -5.694151    -1.230459    -0.455707     102.47
 H      -5.132876    -0.790461     0.406334      21.10
 C      -3.248972    -2.170944    -0.771859      72.23
 H      -2.747027    -2.475169    -1.790986      24.26
 C      -3.589408    -3.338390     0.244613     103.99
 O      -3.745110    -4.736030    -0.161192     304.87
 H      -2.980021    -4.943191    -0.554800      34.27
 H      -4.538678    -2.891135     0.564285      25.01
 H      -2.831480    -2.958838     1.037415      25.57
 C       0.976950    -1.757139    -0.471860      48.84
 H       1.337142    -2.656376    -0.822422      23.03
 C       0.766376     0.198856     0.809240      43.48
 H       1.527498     0.883938     1.467716      17.35
 C      -0.685580     0.042254     0.997645      27.86
 O      -1.556590     0.996712     1.423065     183.53
 C      -0.943761     2.044620     2.167498     119.59
 H      -0.413646     2.872280     1.325560      23.45
 H      -1.672358     2.789223     2.608095      25.48
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 H      -0.311023     2.008569     3.210714      24.03
 C      -1.198880    -1.035943     0.157737      23.29
 O      -2.582731    -0.946470     0.006357     125.47
 C      -0.385644    -1.974575    -0.389390      59.92
 H      -0.974214    -2.955647    -0.871057      16.48
 C       1.675984    -0.610994    -0.009716      42.69
 C       3.104114    -0.416959    -0.027655      81.88
 H       3.709917    -0.595309    -1.104455      21.52
 O       3.308131     1.014403     0.370703     217.44
 H       3.580639     1.111345     1.321450      25.32
 C       3.923336    -1.446130     0.896935      69.56
 H       3.854883    -0.972137     2.173987      20.81
 O       3.527825    -2.845776     0.721787     302.32
 H       3.622521    -3.226974     1.545332      30.21
 C       5.453036    -1.408531     0.903937      90.39
 O       6.075004     0.006939     1.288621     143.83
 H       5.790753    -0.037947     2.301163      27.39
 H       5.961488    -1.797204     0.064394      30.74
 H       5.813695    -2.210382     1.712553      30.25
55
name= lig-ACN-Water-frame_1000
 C      -4.436683    -1.058307    -3.851673      37.09
 H      -5.051800    -1.948600    -3.953721      26.82
 C      -3.678374     0.585927    -2.139269      46.33
 H      -3.775525     0.905930    -0.976795      21.65
 C      -3.404821     1.516973    -3.191151      25.63
 O      -2.856930     2.686739    -2.790584     211.14
 C      -3.598455     3.389907    -1.636642     105.76
 H      -3.370947     4.539831    -1.808658      25.40
 H      -2.990833     3.295292    -0.618840      24.13
 H      -4.610628     2.925205    -1.508819      26.24
 C      -3.554400     1.142517    -4.460193      37.37
 O      -3.217311     2.034736    -5.582202     200.68
 H      -2.882746     2.909671    -5.168071      22.50
 C      -3.993893    -0.116273    -4.822903      55.79
 H      -4.304493    -0.301965    -5.846912      18.32
 C      -4.163467    -0.672104    -2.495146      10.98
 C      -4.551083    -1.667984    -1.414615      94.20
 H      -4.903588    -2.487931    -1.980315      28.96
 O      -5.581609    -1.321701    -0.429423     211.79
 H      -5.195406    -0.636078     0.289475      22.78
 C      -3.177782    -2.227509    -0.762130      68.76
 H      -2.282436    -2.611970    -1.371595      24.28
 C      -3.603206    -3.296782     0.351228     107.77
 O      -3.735586    -4.597708    -0.196601     273.58
 H      -2.944438    -4.768865    -0.735620      30.21
 H      -4.589395    -3.199349     0.866773      23.63
 H      -2.801196    -3.462094     1.247840      26.16
 C       0.999478    -1.816460    -0.521922      51.61
 H       1.816103    -2.391546    -0.951942      17.38
 C       0.678127     0.187552     0.904705      70.91
 H       0.904877     1.237524     1.482130      20.38
 C      -0.664013    -0.007359     0.880053      17.48
 O      -1.663813     1.014859     1.556241     131.27
 C      -0.989506     2.132111     2.167899      85.32
 H      -0.163043     2.779036     1.413015      23.47
 H      -1.921056     2.640253     2.458477      23.94
 H      -0.289984     1.502671     3.028641      22.85
 C      -1.236661    -1.055121     0.176775      31.11
 O      -2.534804    -1.090335    -0.053159     170.67
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 C      -0.356913    -2.116398    -0.407953      88.54
 H      -0.577990    -3.117607    -0.856846      20.93
 C       1.454811    -0.589480     0.037052      28.64
 C       3.077158    -0.270428    -0.125078      64.56
 H       3.071917    -0.145132    -1.371877      21.58
 O       3.505429     1.007394     0.343939     219.82
 H       3.546707     1.012074     1.342683      26.60
 C       3.881063    -1.366273     0.909984      75.41
 H       3.120811    -0.906081     1.877333      21.26
 O       3.643801    -2.787639     0.728415     297.11
 H       3.567308    -3.310098     1.536795      31.28
 C       5.443127    -1.331531     0.954780      93.35
 O       6.102068    -0.093105     1.291067     242.00
 H       6.083828     0.246649     2.216382      29.20
 H       5.779004    -1.533693    -0.107979      27.36
 H       5.767821    -2.041171     1.842985      27.12
55
name= lig-ACN-Water-frame_1001
 C      -4.434546    -1.000705    -3.716645      57.12
 H      -4.874689    -1.893363    -4.110586      24.59
 C      -3.605621     0.578535    -2.199166      54.50
 H      -3.260976     0.918969    -1.137894      24.13
 C      -3.372838     1.518779    -3.165009      -5.68
 O      -2.834117     2.774995    -2.700396     219.33
 C      -3.580876     3.392706    -1.650617     114.60
 H      -3.683626     4.447840    -2.073522      26.29
 H      -3.176885     3.258512    -0.563221      24.40
 H      -4.759500     3.251191    -1.754302      25.27
 C      -3.575654     1.178258    -4.660334      13.27
 O      -3.188717     1.953452    -5.693534     145.13
 H      -3.003416     2.820473    -5.311079      23.44
 C      -4.053741    -0.198954    -4.811861      48.99
 H      -4.248178    -0.512077    -5.771969      21.00
 C      -4.202044    -0.694532    -2.393168      35.84
 C      -4.515339    -1.784751    -1.369569     100.34
 H      -5.038279    -2.605065    -1.812478      26.17
 O      -5.447997    -1.370949    -0.420080     272.18
 H      -5.105169    -0.709562     0.130952      29.26
 C      -3.262226    -2.305023    -0.576323     100.12
 H      -2.774701    -2.822932    -1.441641      25.58
 C      -3.545027    -3.280570     0.475967      94.11
 O      -3.777368    -4.519855    -0.267157     206.83
 H      -2.914215    -4.760916    -0.925385      24.18
 H      -4.473728    -2.903959     1.057084      23.14
 H      -2.565172    -3.169705     1.263127      24.58
 C       1.104079    -1.773543    -0.521537      57.00
 H       1.772688    -2.341922    -1.254221      22.70
 C       0.620875     0.262243     0.935099      58.57
 H       1.295748     1.191853     1.264295      20.66
 C      -0.830801     0.067398     0.841202       6.03
 O      -1.673459     0.854619     1.531315     108.78
 C      -1.071885     2.159987     2.235854      77.68
 H      -0.484770     2.660437     1.261272      24.17
 H      -1.642438     2.962966     2.686972      25.68
 H      -0.305480     1.853927     3.270937      22.83
 C      -1.197809    -1.222829     0.134992      14.15
 O      -2.630325    -1.196881    -0.090672     149.69
 C      -0.290932    -2.180770    -0.377651      55.95
 H      -0.747573    -3.019054    -0.600227      20.52
 C       1.456518    -0.573649     0.146441      29.46
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 C       2.980019    -0.247136    -0.088396      70.26
 H       3.485495    -0.514976    -1.229689      23.12
 O       3.663524     1.023687     0.307622     213.55
 H       3.441290     1.134570     1.284497      27.46
 C       3.774437    -1.254982     0.868456      87.86
 H       3.465806    -1.152030     2.092193      23.18
 O       3.706286    -2.724845     0.672480     210.37
 H       3.587829    -3.089033     1.704944      25.12
 C       5.390003    -1.227996     1.033358      93.91
 O       6.183244    -0.082524     1.300746     236.56
 H       6.018516    -0.007798     2.210384      31.92
 H       5.728711    -1.603177    -0.029802      28.29
 H       5.655222    -2.238440     1.537683      29.82
55
name= lig-ACN-Water-frame_1002
 C      -4.440586    -1.006249    -3.728563      24.80
 H      -4.701647    -2.041097    -3.832666      22.79
 C      -3.558815     0.544851    -2.158786      30.01
 H      -3.031078     0.753537    -1.242691      23.18
 C      -3.321439     1.523181    -3.239701      -3.35
 O      -2.799353     2.792945    -2.733690     186.83
 C      -3.662224     3.533193    -1.725039     107.57
 H      -3.469199     4.598674    -1.512179      25.91
 H      -3.267441     3.049721    -0.749028      24.42
 H      -4.663485     2.877844    -1.755589      23.49
 C      -3.547289     1.137350    -4.592084      13.20
 O      -3.160412     1.894783    -5.775772     199.49
 H      -3.259297     2.845850    -5.598837      24.26
 C      -4.135073    -0.126112    -4.873758      54.17
 H      -4.055096    -0.569344    -5.778156      24.51
 C      -4.206820    -0.736078    -2.341834       9.69
 C      -4.486170    -1.871132    -1.300345      98.79
 H      -4.853491    -2.726147    -1.887448      25.44
 O      -5.476295    -1.346757    -0.335156     233.95
 H      -5.047313    -0.830770     0.288689      28.16
 C      -3.323928    -2.394947    -0.622925      81.98
 H      -2.557890    -2.817135    -1.272071      24.82
 C      -3.519777    -3.362759     0.554757     106.28
 O      -3.874083    -4.510976    -0.238826     183.41
 H      -2.823717    -4.770549    -0.659254      23.50
 H      -4.418644    -3.176390     1.247366      23.46
 H      -2.484406    -3.389923     1.176936      25.42
 C       1.065634    -1.694315    -0.452948      37.88
 H       1.746241    -2.463223    -1.015471      21.60
 C       0.589762     0.285718     0.808320      70.87
 H       0.866132     1.119644     1.552534      21.54
 C      -0.735558     0.008647     0.819122      17.23
 O      -1.755986     0.816759     1.571115     120.67
 C      -1.154640     2.061885     2.204686      94.52
 H      -0.599932     2.780421     1.395286      23.62
 H      -2.163961     2.331259     2.427694      23.84
 H      -0.219153     1.874848     3.112401      21.83
 C      -1.240111    -1.159621     0.186160      18.23
 O      -2.597963    -1.176926    -0.030741     118.68
 C      -0.234168    -2.133509    -0.309228      64.19
 H      -0.352624    -3.011902    -0.778679      18.19
 C       1.598354    -0.537640     0.128830      49.97
 C       3.096477    -0.347580     0.118152      72.71
 H       3.277625    -0.609691    -1.142343      20.80
 O       3.676663     1.024911     0.255362     240.69
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 H       3.541123     1.417488     1.167002      26.27
 C       3.838225    -1.232740     1.014562      92.11
 H       3.333285    -0.770987     2.031146      21.36
 O       3.664252    -2.657660     0.592713     261.26
 H       3.634426    -3.260841     1.424969      28.74
 C       5.312744    -1.232050     0.899952      97.80
 O       6.254610    -0.013570     1.397375     156.81
 H       6.186772     0.209192     2.392564      29.34
 H       5.824833    -1.494743    -0.176377      26.90
 H       5.567297    -1.781971     1.811102      27.62
55
name= lig-ACN-Water-frame_1003
 C      -4.438521    -1.053475    -3.802157      58.60
 H      -4.891724    -1.955449    -4.203571      23.66
 C      -3.509411     0.533692    -2.146941      57.65
 H      -3.389980     0.804271    -1.184905      20.85
 C      -3.293152     1.508400    -3.154587       4.82
 O      -2.792294     2.806460    -2.885415     170.89
 C      -3.674025     3.443991    -1.717342      91.61
 H      -3.435291     4.388629    -2.107467      25.69
 H      -3.390268     3.197977    -0.657929      24.15
 H      -4.877238     3.711262    -2.001629      23.32
 C      -3.518859     1.153114    -4.565766      17.49
 O      -3.156791     1.820271    -5.749944     155.90
 H      -3.435493     2.799189    -5.636290      24.37
 C      -4.142554    -0.123854    -4.779135      58.97
 H      -4.383657    -0.284715    -5.800804      22.82
 C      -4.125565    -0.700494    -2.455435      24.41
 C      -4.583422    -1.763930    -1.278989      78.45
 H      -5.200029    -2.574850    -1.753863      23.82
 O      -5.552779    -1.379468    -0.287657     223.41
 H      -5.231178    -0.674393     0.323899      25.20
 C      -3.123669    -2.317406    -0.532728      85.56
 H      -2.493891    -2.766172    -1.253683      25.01
 C      -3.531845    -3.447317     0.511598     106.17
 O      -3.958178    -4.645485    -0.133953     233.49
 H      -3.200740    -5.131658    -0.719096      26.85
 H      -4.264056    -3.183462     1.390698      23.63
 H      -2.465533    -3.598543     1.048292      23.69
 C       1.105182    -1.667992    -0.359152      31.80
 H       1.921194    -2.409659    -0.689613      15.20
 C       0.684813     0.355974     0.766197      71.54
 H       1.040790     1.198834     1.334670      19.75
 C      -0.710673    -0.049465     0.858038      18.64
 O      -1.692213     0.748672     1.541999     188.40
 C      -1.379263     1.930046     2.123568     111.83
 H      -1.026699     2.770309     1.395772      23.28
 H      -2.033692     2.505512     2.806574      24.28
 H      -0.566283     1.604931     3.155251      22.05
 C      -1.231884    -1.138567     0.183545      26.49
 O      -2.610544    -1.171891     0.061486     222.99
 C      -0.297868    -1.999704    -0.299780      69.04
 H      -0.670120    -2.937624    -0.749776      17.35
 C       1.622054    -0.455811     0.152910      64.91
 C       3.191142    -0.290139     0.134040      49.05
 H       3.724813    -0.760783    -0.994628      18.92
 O       3.609349     1.017085     0.206516     262.55
 H       3.510902     1.253201     1.172296      23.49
 C       3.933176    -1.290350     1.179233      98.77
 H       3.789501    -1.536231     2.308749      22.48
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 O       3.538917    -2.577717     0.570850     320.63
 H       3.836700    -3.225488     1.116767      34.05
 C       5.529301    -1.129559     1.037966      87.46
 O       6.228963     0.049471     1.438580     254.09
 H       5.995850    -0.038446     2.479438      26.45
 H       5.629644    -1.334280    -0.227261      28.88
 H       5.916090    -2.147161     1.289165      32.41
55
name= lig-ACN-Water-frame_1004
 C      -4.424296    -1.073762    -3.820559      40.78
 H      -5.121222    -1.921502    -3.982924      22.53
 C      -3.551831     0.546621    -2.164808      44.43
 H      -3.595418     0.873972    -1.219898      22.35
 C      -3.218012     1.476140    -3.179847      14.20
 O      -2.923127     2.790612    -2.922361     227.47
 C      -3.570133     3.513113    -1.925728     105.92
 H      -3.169767     4.463516    -1.735847      27.04
 H      -3.440761     3.068096    -0.905494      26.08
 H      -4.825272     3.153413    -2.139071      23.13
 C      -3.494628     1.108544    -4.488073      31.14
 O      -3.172614     1.795623    -5.641136     196.00
 H      -3.314846     2.753393    -5.561999      26.33
 C      -4.121763    -0.098442    -4.803169      51.13
 H      -4.640722    -0.171477    -5.808944      22.88
 C      -4.142276    -0.780450    -2.456780      19.78
 C      -4.513843    -1.655325    -1.289960      92.42
 H      -4.816366    -2.615640    -1.825299      26.76
 O      -5.619018    -1.386984    -0.274551     164.37
 H      -5.293969    -0.503230     0.270411      22.92
 C      -3.273689    -2.286218    -0.543229      93.34
 H      -2.661018    -2.452338    -1.377192      28.87
 C      -3.423989    -3.483419     0.427079     115.27
 O      -4.059651    -4.818089    -0.025183     239.74
 H      -3.394956    -5.032010    -0.583828      34.97
 H      -4.283551    -2.960338     1.000853      24.14
 H      -2.505138    -3.623063     1.024652      27.42
 C       1.123417    -1.714774    -0.289329      25.83
 H       1.627933    -2.537375    -0.810684      21.68
 C       0.729385     0.499027     0.850141      93.74
 H       1.047490     1.473479     0.943167      22.44
 C      -0.613402     0.107446     0.928687      20.85
 O      -1.744759     0.625606     1.463890     150.69
 C      -1.496401     1.920062     2.207800     100.68
 H      -1.101587     2.662883     1.366328      24.10
 H      -2.543485     2.055987     2.531954      23.55
 H      -0.378789     1.904899     2.818175      22.10
 C      -1.167660    -1.052494     0.227751       4.71
 O      -2.616308    -1.168536     0.209396     120.85
 C      -0.251028    -1.976026    -0.418492      76.91
 H      -0.628400    -3.070053    -0.792923      23.23
 C       1.674054    -0.515737     0.159500      58.77
 C       3.183154    -0.302274     0.197188      51.12
 H       3.685836    -0.851761    -0.898010      21.14
 O       3.572565     1.101047     0.228793     209.37
 H       3.534356     1.398744     1.212034      25.23
 C       4.092571    -1.394097     1.273499      60.11
 H       3.610626    -1.060026     2.248860      25.05
 O       3.494757    -2.532993     0.591397     289.77
 H       3.870788    -3.430701     1.015467      31.72
 C       5.692662    -1.198862     1.011485      88.10
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 O       6.149294     0.096036     1.568903     175.90
 H       6.282188     0.213026     2.558534      29.77
 H       5.779960    -0.719045    -0.150491      29.64
 H       6.479309    -1.886959     1.301912      29.09
55
name= lig-ACN-Water-frame_1005
 C      -4.456496    -1.054496    -3.745098      47.25
 H      -4.965046    -2.023929    -4.017424      19.86
 C      -3.665151     0.537600    -2.144909      79.38
 H      -3.407623     0.754695    -1.129422      30.05
 C      -3.247338     1.406976    -3.157277       6.54
 O      -2.916364     2.802192    -3.070215     199.57
 C      -3.565803     3.497191    -1.963011     108.76
 H      -3.201539     4.487889    -2.039555      27.74
 H      -3.333796     2.984435    -1.037800      26.48
 H      -4.865398     3.885370    -2.084405      23.49
 C      -3.457981     1.000426    -4.530440       1.90
 O      -3.170990     1.880477    -5.560516     157.57
 H      -3.014652     2.724274    -5.119819      24.06
 C      -4.179443    -0.184364    -4.817474      51.83
 H      -4.308609    -0.405087    -5.999411      22.55
 C      -4.160287    -0.705375    -2.398531      33.25
 C      -4.526745    -1.744508    -1.259142      81.70
 H      -5.031410    -2.630681    -1.769130      24.10
 O      -5.613845    -1.348759    -0.377420     105.19
 H      -5.264762    -0.580278     0.355715      22.32
 C      -3.263049    -2.242179    -0.666300      66.30
 H      -2.572515    -2.600556    -1.385262      27.78
 C      -3.517097    -3.485919     0.399165     109.23
 O      -4.026312    -4.844991     0.075200     211.13
 H      -3.551054    -5.389424    -0.525309      31.33
 H      -4.096135    -3.328534     1.383743      24.30
 H      -2.515346    -3.594837     0.699430      27.67
 C       1.130358    -1.760019    -0.326150      33.11
 H       1.912871    -2.302260    -0.716717      18.13
 C       0.839179     0.490823     0.797150      61.05
 H       1.037315     1.467644     1.109595      21.36
 C      -0.610467     0.082914     0.820707      -1.32
 O      -1.771784     0.718636     1.536548     154.58
 C      -1.612587     1.912312     2.152528     128.40
 H      -1.746346     2.856337     1.571841      27.67
 H      -2.466678     2.072335     2.917099      25.36
 H      -0.980358     1.878507     3.250584      23.76
 C      -1.107701    -1.063615     0.207761      35.02
 O      -2.529196    -1.194216     0.372435      46.92
 C      -0.271664    -1.927900    -0.425433      55.72
 H      -0.569181    -2.931012    -1.125255      23.70
 C       1.649859    -0.527218     0.331316      27.47
 C       3.278180    -0.325028     0.256878      65.12
 H       3.445948    -0.438585    -1.015634      19.94
 O       3.572479     1.108750     0.274632     273.27
 H       3.516766     1.462390     1.268047      20.24
 C       4.155041    -1.316165     1.132133      88.41
 H       4.080502    -1.291671     2.275666      22.13
 O       3.568471    -2.582042     0.719292     282.76
 H       3.795892    -3.557383     1.167205      29.08
 C       5.710869    -1.134472     0.962430      84.57
 O       6.129293     0.186243     1.711860     247.55
 H       5.994566    -0.120707     2.630322      27.45
 H       5.974262    -1.388964    -0.226268      29.33
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 H       6.106500    -2.059054     1.387164      32.05
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name= lig-ACN-Water-frame_1006
 C      -4.525410    -1.076437    -3.713527      66.81
 H      -4.800937    -2.147675    -3.912753      24.22
 C      -3.666903     0.627637    -2.040511      30.75
 H      -3.400246     0.974132    -0.958884      23.32
 C      -3.377078     1.390437    -3.223979      -8.19
 O      -2.908649     2.741358    -3.203335     151.07
 C      -3.542229     3.571654    -1.962466      79.48
 H      -2.930699     4.443783    -2.090585      27.11
 H      -3.427503     3.280528    -0.927028      24.95
 H      -4.860600     3.581880    -2.324366      21.32
 C      -3.481246     0.950396    -4.581416       1.09
 O      -3.151024     1.979237    -5.486359     117.76
 H      -2.762730     2.727071    -4.917371      20.46
 C      -4.128651    -0.278182    -4.814438      55.34
 H      -4.264874    -0.896411    -5.871862      21.11
 C      -4.304214    -0.730241    -2.377033       6.54
 C      -4.590166    -1.742061    -1.349310      79.04
 H      -4.944685    -2.707826    -1.837522      26.56
 O      -5.589627    -1.285883    -0.463634     181.22
 H      -5.195226    -0.668157     0.228992      24.30
 C      -3.177943    -2.345868    -0.485972      81.45
 H      -2.520507    -2.523795    -1.343326      30.53
 C      -3.445361    -3.520948     0.443512     122.17
 O      -4.035559    -4.822488     0.129901     192.74
 H      -3.072320    -5.076988    -0.418033      25.74
 H      -3.965559    -2.978073     1.254018      26.43
 H      -2.491539    -3.758992     0.753817      28.29
 C       1.199618    -1.632703    -0.308805      47.26
 H       1.692238    -2.395352    -0.760172      25.51
 C       0.690401     0.380408     0.790741      75.53
 H       1.229753     1.182593     1.297081      22.51
 C      -0.670288     0.155639     0.804052      30.24
 O      -1.670636     0.758334     1.509423     150.50
 C      -1.804277     2.060623     2.336694     118.37
 H      -1.540647     2.899318     1.630955      26.37
 H      -2.860414     1.991059     2.767281      23.61
 H      -0.688444     2.032163     2.705799      22.09
 C      -1.155147    -1.084393     0.182807       7.25
 O      -2.510905    -1.348968     0.360732     147.78
 C      -0.183896    -1.950946    -0.463432      44.99
 H      -0.762887    -2.819255    -1.142068      22.72
 C       1.752855    -0.603665     0.418805      42.68
 C       3.242244    -0.287623     0.222406      85.02
 H       3.620552    -0.832124    -0.866714      22.38
 O       3.620878     1.042479     0.292207     283.60
 H       3.556363     1.317381     1.304106      22.31
 C       4.154420    -1.216952     1.003644      68.86
 H       3.904111    -0.947417     2.106782      22.84
 O       3.698996    -2.675331     0.831181     291.44
 H       4.040759    -2.854795     1.679596      29.04
 C       5.670023    -1.070156     1.002212     104.38
 O       6.116387     0.118377     1.649733     281.07
 H       6.111780     0.094262     2.586104      32.98
 H       6.378876    -0.829557     0.049231      29.07
 H       6.082111    -1.846561     1.628104      32.16
55
name= lig-ACN-Water-frame_1007
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 C      -4.517488    -1.096397    -3.698506      40.14
 H      -5.020335    -2.066385    -3.851389      23.63
 C      -3.749783     0.568101    -2.147133      74.64
 H      -3.646460     1.061610    -1.046823      22.71
 C      -3.497953     1.404826    -3.210171      22.28
 O      -2.969815     2.699356    -3.093113     231.74
 C      -3.429415     3.606176    -2.146097     121.55
 H      -3.134087     4.689121    -2.121600      25.86
 H      -3.247250     3.020707    -1.253886      25.91
 H      -4.805914     3.748775    -2.288035      23.89
 C      -3.584205     0.997232    -4.575692      12.23
 O      -3.125368     1.964712    -5.481639     127.85
 H      -2.949130     2.760538    -4.870988      21.01
 C      -4.034495    -0.377347    -4.838830      43.57
 H      -4.160968    -0.667111    -6.016950      14.79
 C      -4.308479    -0.623258    -2.349727      37.09
 C      -4.472102    -1.792600    -1.274884      78.27
 H      -4.899846    -2.665363    -1.840719      26.61
 O      -5.623775    -1.227962    -0.463437     181.16
 H      -5.221693    -0.722471     0.169278      31.50
 C      -3.208350    -2.411466    -0.523281      93.48
 H      -2.528737    -2.885745    -1.306414      27.66
 C      -3.316036    -3.521976     0.661770     102.12
 O      -3.991159    -4.746626     0.101193     154.89
 H      -3.419551    -5.547269    -0.459603      26.32
 H      -4.080190    -3.290136     1.344882      26.43
 H      -2.462189    -3.602322     1.238890      28.95
 C       1.198314    -1.728249    -0.375138      22.11
 H       1.982265    -2.261444    -0.836400      20.42
 C       0.742979     0.307241     0.927045      71.93
 H       0.780700     1.320380     1.396005      19.75
 C      -0.702111     0.089144     0.798330       4.92
 O      -1.731556     0.857354     1.498446     133.23
 C      -1.721061     2.146463     2.336338     116.74
 H      -2.131879     2.910555     1.736185      27.45
 H      -2.651874     1.886639     2.973215      24.51
 H      -1.274489     2.415515     3.407072      23.43
 C      -1.162049    -1.087197     0.155423      28.53
 O      -2.528934    -1.469541     0.299256     173.77
 C      -0.170901    -1.866003    -0.436548      63.21
 H      -0.185671    -2.974254    -0.846087      24.88
 C       1.670450    -0.564372     0.335969      23.71
 C       3.206106    -0.384504     0.069469      71.41
 H       3.157580    -0.306355    -1.150313      21.91
 O       3.689259     1.014568     0.262482     215.11
 H       3.582865     1.458419     1.206556      24.51
 C       4.090402    -1.215253     1.094438      92.96
 H       3.726229    -0.766421     2.074035      23.43
 O       3.911465    -2.654449     1.000553     331.13
 H       3.820758    -3.223379     1.721094      33.17
 C       5.703329    -1.060023     1.020309      94.36
 O       6.165961     0.179206     1.618792     252.43
 H       5.973605    -0.007269     2.506383      32.25
 H       5.811208    -1.198764    -0.161806      29.47
 H       6.117981    -1.985747     1.338287      32.20
55
name= lig-ACN-Water-frame_1008
 C      -4.445814    -1.112237    -3.744345      53.83
 H      -4.966778    -2.022832    -3.991104      28.27
 C      -3.861096     0.609532    -2.158295      30.53
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 H      -3.629172     0.881722    -0.986438      30.11
 C      -3.595862     1.473447    -3.218967       6.43
 O      -2.945491     2.680592    -3.094603     197.35
 C      -3.459915     3.638606    -2.133612      99.08
 H      -2.752208     4.422013    -2.640248      24.33
 H      -3.216672     3.694540    -1.079651      25.29
 H      -4.783659     3.921739    -2.232800      22.15
 C      -3.653644     1.003712    -4.565999      32.60
 O      -3.134447     1.865835    -5.521729     195.18
 H      -3.200877     2.748010    -5.170138      26.59
 C      -3.990266    -0.288374    -4.815143      63.17
 H      -4.071167    -0.736512    -5.865168      17.61
 C      -4.224002    -0.838068    -2.388646      -1.62
 C      -4.472811    -1.767592    -1.188247      84.00
 H      -4.984823    -2.655113    -1.608778      25.48
 O      -5.598010    -1.230078    -0.401149     152.55
 H      -5.296371    -0.806733     0.430892      25.65
 C      -3.207059    -2.517596    -0.494796      62.88
 H      -2.652089    -3.027090    -1.384539      25.99
 C      -3.423538    -3.578704     0.727520     118.39
 O      -3.939869    -4.709737     0.104681     238.97
 H      -3.163369    -5.105383    -0.328484      30.44
 H      -4.011021    -3.169096     1.462448      26.88
 H      -2.403908    -3.773370     0.953361      26.87
 C       1.219769    -1.680089    -0.385766      65.90
 H       1.803317    -2.468601    -0.911980      23.08
 C       0.684224     0.312688     1.041637      83.47
 H       1.360444     1.129134     1.500295      20.56
 C      -0.668524     0.041617     0.905165      10.97
 O      -1.765002     0.958925     1.489048     131.49
 C      -1.788287     2.130657     2.361972     112.58
 H      -1.905384     3.013138     1.804997      28.57
 H      -2.660207     1.944723     3.053181      25.42
 H      -0.549051     2.212442     2.623135      23.27
 C      -1.159202    -1.108640     0.133508      14.69
 O      -2.476049    -1.394307     0.241005     118.14
 C      -0.217896    -2.024059    -0.450631      61.24
 H      -0.836437    -2.835588    -0.804288      23.60
 C       1.635492    -0.480859     0.191259      40.56
 C       3.146438    -0.287497     0.025748      59.40
 H       3.639242    -0.875789    -0.908433      24.07
 O       3.728406     1.007102     0.195747     214.03
 H       3.419295     1.232301     1.111117      27.19
 C       4.114530    -1.281586     1.254253      61.15
 H       3.814667    -0.968344     2.280371      24.79
 O       4.062316    -2.675894     1.107583     256.18
 H       3.692308    -2.960050     2.097861      24.89
 C       5.575881    -1.053084     0.930742      95.20
 O       6.257740     0.209255     1.609531     130.04
 H       5.877943     0.358152     2.550814      30.61
 H       5.898533    -0.850218    -0.128009      30.32
 H       6.144417    -1.839850     1.414069      29.46
55
name= lig-ACN-Water-frame_1009
 C      -4.338466    -1.249717    -3.791427      33.90
 H      -4.465886    -2.245398    -4.141658      27.42
 C      -3.948427     0.492893    -2.112585      39.57
 H      -3.662461     0.982475    -1.073516      32.72
 C      -3.671093     1.434843    -3.177234     -37.69
 O      -2.941856     2.661321    -3.073606     131.12
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 C      -3.419242     3.863564    -2.120210      83.34
 H      -3.125173     4.985432    -2.428058      24.16
 H      -3.184079     3.463059    -1.110919      25.65
 H      -4.723777     3.735120    -2.402681      20.25
 C      -3.652879     1.058109    -4.521355      18.03
 O      -3.156462     1.762659    -5.640971     141.18
 H      -3.281860     2.733472    -5.490554      25.49
 C      -4.073748    -0.269695    -4.808448      38.08
 H      -3.996528    -0.604417    -5.810365      24.01
 C      -4.116232    -0.844653    -2.384381     -39.54
 C      -4.571408    -1.863716    -1.182531      69.17
 H      -5.013895    -2.733532    -1.651492      23.41
 O      -5.529448    -1.250255    -0.263313     138.33
 H      -4.878921    -0.672491     0.431129      20.45
 C      -3.261789    -2.393089    -0.344844      90.53
 H      -2.570893    -2.841409    -1.177555      26.05
 C      -3.459919    -3.480064     0.642497     125.79
 O      -3.929319    -4.806317     0.101436     209.97
 H      -3.359063    -5.188407    -0.523934      30.68
 H      -4.071628    -3.247409     1.453837      27.04
 H      -2.557626    -3.627049     1.258944      26.73
 C       1.046260    -1.684489    -0.457213      46.50
 H       1.918506    -2.259270    -0.938675      22.22
 C       0.773377     0.290237     0.974380      68.68
 H       0.976228     1.117772     1.796618      22.16
 C      -0.688618     0.132897     1.074456       0.18
 O      -1.805824     0.880557     1.360652     160.04
 C      -1.649407     2.096877     2.316786     108.90
 H      -1.927798     2.883996     1.691593      28.56
 H      -2.157904     2.155299     3.293254      27.92
 H      -0.518636     2.085073     2.881010      24.32
 C      -1.089771    -1.100744     0.223985      -3.80
 O      -2.493433    -1.282578     0.148614     101.73
 C      -0.250035    -2.095901    -0.403398      84.29
 H      -0.323917    -2.905510    -0.972070      25.35
 C       1.626402    -0.475741     0.107933      35.63
 C       3.216850    -0.354895     0.237315      75.56
 H       3.555168    -0.767498    -0.837518      23.85
 O       3.700042     1.032583     0.122355     220.40
 H       3.737347     1.514300     0.942547      28.85
 C       4.115598    -1.199753     1.282374      81.90
 H       3.948271    -0.865823     2.309821      26.42
 O       4.081241    -2.768375     1.220886     227.85
 H       3.867932    -3.291557     2.125804      27.22
 C       5.643734    -0.846636     0.985901     106.58
 O       6.282174     0.197535     1.562084     173.96
 H       5.888375     0.291173     2.569861      29.54
 H       5.732188    -0.795265    -0.124020      31.80
 H       6.060978    -1.841346     1.186363      30.85
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name= lig-ACN-Water-frame_1010
 C      -4.138226    -1.311704    -3.747964      41.05
 H      -4.200664    -2.358783    -3.940098      22.18
 C      -3.922892     0.496989    -2.116724      37.83
 H      -4.072445     0.704174    -1.042083      21.27
 C      -3.633601     1.475507    -3.123272     -21.03
 O      -2.950230     2.776489    -2.965449     196.88
 C      -3.466019     3.853928    -2.190136      99.89
 H      -2.886790     4.877186    -2.473735      25.37
 H      -3.118525     3.760704    -1.060872      25.54
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 H      -4.786668     4.060183    -2.011527      23.13
 C      -3.717508     0.972696    -4.534234     -13.54
 O      -3.202674     1.684707    -5.732673     115.58
 H      -3.244818     2.676848    -5.496592      22.31
 C      -4.130869    -0.346865    -4.814073      62.67
 H      -4.187625    -0.522706    -5.788014      27.43
 C      -4.230194    -0.934839    -2.397462      16.13
 C      -4.528521    -1.874584    -1.161712      99.16
 H      -5.088024    -2.732381    -1.472774      27.28
 O      -5.435070    -1.289021    -0.163807     171.23
 H      -4.927921    -0.638388     0.662136      16.44
 C      -3.255114    -2.271594    -0.456873      84.10
 H      -2.596102    -2.822288    -1.238493      25.83
 C      -3.509621    -3.463379     0.701883      89.12
 O      -3.927337    -4.863701     0.115867     112.81
 H      -3.348085    -5.226555    -0.747551      26.97
 H      -4.490477    -3.299037     1.051494      24.33
 H      -2.563140    -3.494266     1.297531      26.10
 C       1.154087    -1.599298    -0.528106      41.92
 H       1.692173    -2.351008    -1.214183      23.53
 C       0.728456     0.351074     0.961811      67.61
 H       1.450339     1.183401     1.384382      20.23
 C      -0.637258    -0.062609     0.913048      20.17
 O      -1.774132     0.861300     1.342011      84.57
 C      -1.439500     2.007645     2.250920     120.89
 H      -1.860310     2.906931     1.829870      27.82
 H      -2.203039     1.674622     2.890567      25.12
 H      -0.295230     2.333893     2.536464      23.47
 C      -1.178735    -1.179616     0.363699      18.31
 O      -2.570373    -1.081162     0.122190     144.13
 C      -0.259661    -2.020042    -0.323667      61.15
 H      -0.708904    -2.833298    -0.603114      23.07
 C       1.620254    -0.539673     0.298502      31.04
 C       3.209986    -0.480104     0.302709      73.85
 H       3.514947    -0.857480    -0.729619      26.23
 O       3.667650     1.069780     0.105506     178.61
 H       3.752921     1.437877     1.034708      26.86
 C       4.163110    -1.167232     1.375650      89.03
 H       3.818231    -0.854631     2.338155      25.68
 O       4.029823    -2.714594     1.274326     254.74
 H       4.269979    -2.985797     2.128299      30.89
 C       5.657553    -0.885945     0.898292      89.94
 O       6.289006     0.317160     1.620443     113.89
 H       6.176070     0.143172     2.576875      32.80
 H       5.687195    -0.578023    -0.085394      33.94
 H       6.365580    -1.762713     1.087474      30.92
55
name= lig-ACN-Water-frame_1011
 C      -4.066712    -1.386328    -3.708265      19.16
 H      -4.248061    -2.418668    -4.033437      20.58
 C      -3.963961     0.510530    -2.135424      51.27
 H      -4.030527     0.935225    -1.195943      24.51
 C      -3.545579     1.470210    -3.161038       3.40
 O      -3.019121     2.751109    -2.925732     197.48
 C      -3.492030     3.876976    -2.108957      92.45
 H      -3.098026     4.713469    -2.814915      24.95
 H      -3.139661     3.914119    -0.963108      24.15
 H      -4.773134     4.004227    -2.455016      23.24
 C      -3.710651     0.965891    -4.558879      15.99
 O      -3.324112     1.603136    -5.674791     171.17
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 H      -3.179449     2.528004    -5.493488      25.99
 C      -4.079851    -0.437945    -4.770941      43.66
 H      -4.232016    -0.898918    -5.651189      28.23
 C      -4.305702    -0.840713    -2.368220      22.27
 C      -4.494583    -1.779512    -1.129206     103.60
 H      -4.870906    -2.705631    -1.533451      29.40
 O      -5.402839    -1.318530    -0.136536     208.68
 H      -4.767028    -0.974438     0.706941      20.66
 C      -3.182617    -2.364249    -0.523855      70.56
 H      -2.444018    -2.597963    -1.346742      28.07
 C      -3.649085    -3.479679     0.600925     109.66
 O      -3.883696    -4.806806     0.132661     205.52
 H      -2.824878    -4.958934    -0.247683      24.17
 H      -4.318891    -2.966280     1.316956      25.80
 H      -2.851843    -3.601144     1.422106      25.86
 C       1.104408    -1.632974    -0.411008      37.34
 H       1.835398    -2.132113    -1.076450      26.49
 C       0.726511     0.282461     0.920363      59.17
 H       0.769126     1.377579     1.231778      24.53
 C      -0.658227     0.054302     0.883045      16.84
 O      -1.566620     0.853519     1.311211     222.08
 C      -1.365188     1.911832     2.185420     141.35
 H      -1.653589     2.882814     1.677941      27.80
 H      -1.573352     1.951486     3.226951      27.66
 H      -0.247398     1.769642     2.396036      24.17
 C      -1.252953    -1.196676     0.377824       7.01
 O      -2.601175    -1.052396     0.073677     106.77
 C      -0.238212    -1.996728    -0.327598      65.22
 H      -0.391888    -2.840090    -0.876111      26.75
 C       1.734768    -0.679633     0.421012      29.94
 C       3.187586    -0.400570     0.252133      88.82
 H       3.486571    -1.034296    -0.568896      29.40
 O       3.601530     0.965799     0.157161     233.84
 H       3.654873     1.359928     1.114749      26.90
 C       4.211515    -1.202121     1.379570      89.86
 H       4.267965    -0.820022     2.372949      28.09
 O       3.961212    -2.535737     1.332356     278.51
 H       4.355305    -3.091157     2.014427      30.79
 C       5.678609    -0.841647     0.904817      85.14
 O       6.253790     0.383932     1.672528      91.86
 H       6.249227     0.126326     2.550003      33.95
 H       5.722201    -0.650370    -0.084809      32.97
 H       6.288767    -1.813335     1.126965      32.01
55
name= lig-ACN-Water-frame_1012
 C      -4.211832    -1.336929    -3.605640      67.67
 H      -4.320284    -2.452979    -3.687401      27.74
 C      -4.024321     0.623082    -2.150423      73.10
 H      -3.886694     0.974277    -1.229785      36.58
 C      -3.589740     1.369233    -3.212087      20.70
 O      -3.023039     2.630699    -2.949993     172.95
 C      -3.583779     3.910514    -2.190136      86.32
 H      -3.138624     4.938976    -2.339281      24.75
 H      -3.303069     3.601691    -1.027239      24.09
 H      -4.880463     3.792294    -1.966861      22.71
 C      -3.676358     0.841467    -4.492755      28.04
 O      -3.440050     1.605103    -5.655547     164.79
 H      -3.264417     2.533669    -5.388337      25.42
 C      -3.923708    -0.511623    -4.685560      59.38
 H      -3.828958    -0.650475    -5.760755      19.60
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 C      -4.214029    -0.769380    -2.319429      -8.99
 C      -4.486238    -1.803877    -1.226982      70.97
 H      -5.120347    -2.542150    -1.684918      23.18
 O      -5.416285    -1.366868    -0.163070     118.43
 H      -5.095485    -0.565825     0.424883      23.54
 C      -3.219792    -2.355102    -0.505768     107.74
 H      -2.605064    -3.016756    -1.145306      28.56
 C      -3.588809    -3.360734     0.596615      96.77
 O      -3.828639    -4.715418     0.105444     149.68
 H      -3.126037    -5.375403    -0.151708      28.30
 H      -4.717304    -3.285998     0.837619      21.56
 H      -2.683389    -3.277152     1.300591      26.93
 C       1.123771    -1.798901    -0.173982      52.97
 H       1.709855    -2.467184    -0.738826      24.20
 C       0.797745     0.226268     0.911619      78.97
 H       1.319073     1.103958     1.274287      25.40
 C      -0.599360    -0.036263     0.865475      21.57
 O      -1.617645     0.925477     1.313123     166.50
 C      -1.108935     1.959157     2.240386     108.62
 H      -1.593990     2.922310     1.750305      27.29
 H      -1.811947     1.705179     2.971899      27.06
 H      -0.044779     2.188923     2.408622      26.63
 C      -1.147853    -1.125051     0.204791      17.63
 O      -2.553898    -1.243862     0.052996     146.86
 C      -0.268743    -2.041073    -0.401117      58.88
 H      -0.564790    -2.772797    -1.150148      24.36
 C       1.684895    -0.632725     0.448122      28.13
 C       3.280712    -0.469878     0.333611     107.88
 H       3.459596    -0.644527    -0.678678      28.53
 O       3.528201     0.914561     0.227669     260.21
 H       3.490492     1.395346     1.085387      28.51
 C       4.276041    -1.030071     1.335106      82.77
 H       3.938189    -0.560932     2.246380      27.88
 O       3.843338    -2.472231     1.348691     222.29
 H       4.312308    -3.067415     2.179267      27.30
 C       5.739651    -0.753396     0.984983     104.44
 O       6.195656     0.350639     1.666715     182.92
 H       6.038504     0.198018     2.681862      29.66
 H       5.869823    -0.563970    -0.012136      31.97
 H       6.420491    -1.681477     1.244661      30.24
55
name= lig-ACN-Water-frame_1013
 C      -4.322941    -1.275686    -3.558696      37.93
 H      -4.559235    -2.396975    -3.660384      27.47
 C      -4.016350     0.631523    -2.018028      69.34
 H      -4.012596     1.051580    -1.063690      28.41
 C      -3.696564     1.441049    -3.158218       3.07
 O      -3.000512     2.668606    -3.042418     167.77
 C      -3.693649     3.679192    -2.158202      88.88
 H      -3.217072     4.444052    -2.817421      24.71
 H      -3.194916     3.600006    -1.013330      23.39
 H      -4.949679     3.912873    -2.445303      22.73
 C      -3.608538     0.815287    -4.530903      19.24
 O      -3.534476     1.630409    -5.625358     148.47
 H      -3.447642     2.576489    -5.237370      21.61
 C      -3.785266    -0.586631    -4.702545      49.80
 H      -3.692228    -1.307137    -5.630787      18.23
 C      -4.194513    -0.770382    -2.240150      15.80
 C      -4.530681    -1.789512    -1.213284      83.45
 H      -4.859416    -2.708107    -1.745638      24.82
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 O      -5.495236    -1.382357    -0.250541     165.90
 H      -5.139588    -0.674431     0.220935      26.76
 C      -3.261968    -2.439176    -0.562054      87.84
 H      -2.693039    -2.840944    -1.399451      28.23
 C      -3.567876    -3.325068     0.627391     110.60
 O      -3.814657    -4.701417     0.071393     192.08
 H      -3.046843    -4.771321    -0.405001      31.92
 H      -4.454269    -2.769828     1.264503      22.10
 H      -2.919784    -3.270402     1.589901      23.65
 C       1.197098    -2.064071    -0.083156      34.97
 H       1.856278    -2.850052    -0.182694      24.63
 C       0.826272     0.311342     0.991628      49.67
 H       1.152313     1.107244     1.551890      20.75
 C      -0.625576     0.032868     0.876747      -5.94
 O      -1.556468     0.962284     1.287672     147.39
 C      -1.042048     2.075139     2.311841      93.23
 H      -1.357849     3.227106     1.977322      24.07
 H      -1.344820     1.922661     3.319695      27.85
 H      -0.045097     1.838476     2.493985      27.10
 C      -1.143470    -1.108632    -0.012367       9.11
 O      -2.470627    -1.328599     0.082984     119.02
 C      -0.150461    -2.117615    -0.471182      60.53
 H      -0.711601    -3.102040    -0.799474      22.89
 C       1.745630    -0.848806     0.388222      10.61
 C       3.237092    -0.489035     0.267444      89.71
 H       3.594360    -1.051292    -0.498845      26.19
 O       3.489686     1.057283     0.296462     194.22
 H       3.400525     1.316272     1.210639      26.59
 C       4.159105    -1.028493     1.338688      78.50
 H       4.106416    -0.549378     2.323467      24.97
 O       3.786628    -2.410844     1.376385     266.52
 H       4.082702    -2.698318     2.362301      26.52
 C       5.762641    -0.798347     1.007811      77.56
 O       6.211098     0.431825     1.753364     163.52
 H       5.924118     0.299895     2.803989      27.43
 H       5.948456    -0.590207     0.009944      31.62
 H       6.318416    -1.802207     1.369491      29.84
55
name= lig-ACN-Water-frame_1014
 C      -4.255610    -1.259596    -3.556892      31.39
 H      -4.750736    -2.257422    -3.790182      21.64
 C      -3.942072     0.611015    -1.965023      57.37
 H      -4.009978     1.086591    -0.951572      20.38
 C      -3.686417     1.361790    -3.161840      -2.08
 O      -3.109560     2.662948    -3.139755     214.41
 C      -3.673966     3.561606    -2.280782     104.77
 H      -3.529719     4.660358    -2.317810      26.21
 H      -3.668103     3.425533    -1.005935      24.36
 H      -4.973966     3.224749    -2.335479      23.74
 C      -3.614063     0.816497    -4.462939       8.82
 O      -3.575165     1.685784    -5.597700     101.08
 H      -3.488739     2.620199    -5.359623      21.66
 C      -3.785976    -0.603801    -4.659460      49.10
 H      -3.621677    -1.126460    -5.768000      19.96
 C      -4.329307    -0.727748    -2.225427      21.35
 C      -4.520186    -1.827841    -1.137331      84.60
 H      -5.107730    -2.619268    -1.688405      24.62
 O      -5.627005    -1.378819    -0.318513     127.38
 H      -5.351164    -0.854681     0.490671      26.16
 C      -3.189717    -2.374262    -0.542069      86.59
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 H      -2.636808    -2.888112    -1.309841      29.48
 C      -3.581873    -3.390597     0.668962     101.90
 O      -3.820797    -4.640384     0.097417     181.57
 H      -3.246012    -4.912104    -0.664585      29.98
 H      -4.620972    -3.103535     1.240257      22.10
 H      -2.555898    -3.541910     1.100244      25.11
 C       1.278077    -2.193037    -0.052267      33.12
 H       1.873068    -3.074142    -0.089611      24.32
 C       0.805197     0.057609     0.898387      78.21
 H       1.251356     0.914255     1.251211      24.39
 C      -0.553285     0.106135     0.730546      20.17
 O      -1.484355     1.073929     1.363870     179.28
 C      -1.007468     2.039561     2.360578     109.83
 H      -1.142165     3.147866     1.751228      23.85
 H      -1.537811     1.942977     3.257860      27.20
 H       0.055752     2.094106     2.386806      27.04
 C      -0.997182    -1.029862    -0.001378     -10.80
 O      -2.457644    -1.306295     0.088116     110.73
 C      -0.098511    -2.219793    -0.415975      56.49
 H      -0.332663    -3.399737    -0.646083      21.04
 C       1.718295    -0.849824     0.422651      22.78
 C       3.205744    -0.344905     0.235834      90.89
 H       3.485147    -0.393110    -0.726689      28.69
 O       3.428003     1.071717     0.276631     189.84
 H       3.393056     1.495057     1.198507      27.59
 C       4.146924    -1.043597     1.391592      83.98
 H       3.871700    -0.548507     2.357219      26.22
 O       3.787346    -2.421186     1.464444     334.17
 H       3.823484    -2.882136     2.230959      33.51
 C       5.667833    -0.802432     1.112416      82.09
 O       6.237836     0.465801     1.828974      99.23
 H       6.097634     0.211977     2.833325      28.16
 H       5.939225    -0.792261     0.010684      28.96
 H       6.243588    -1.709167     1.580108      29.64
55
name= lig-ACN-Water-frame_1015
 C      -4.211689    -1.320017    -3.523127      28.45
 H      -4.389405    -2.415687    -3.585140      21.86
 C      -3.915981     0.566577    -2.046317      47.55
 H      -3.733692     0.990608    -0.941678      25.06
 C      -3.535951     1.308551    -3.137893      22.49
 O      -3.180859     2.637337    -3.273365     192.43
 C      -3.885329     3.507703    -2.200910      82.98
 H      -3.472413     4.468798    -2.531959      25.88
 H      -3.221454     3.003570    -1.345548      22.69
 H      -5.219267     3.524186    -2.316040      22.41
 C      -3.668625     0.854074    -4.478479      32.87
 O      -3.575072     1.676757    -5.547460     136.93
 H      -3.412411     2.514829    -5.085145      23.47
 C      -3.844653    -0.465253    -4.645661      45.88
 H      -3.830306    -0.764341    -5.838531      19.46
 C      -4.382895    -0.772924    -2.247828      37.30
 C      -4.569225    -1.750274    -1.181304      83.07
 H      -4.783389    -2.783912    -1.593237      27.06
 O      -5.737503    -1.356110    -0.260315      82.19
 H      -5.294836    -1.055980     0.664575      26.13
 C      -3.221003    -2.281755    -0.379350      97.70
 H      -2.635938    -2.772667    -1.148364      30.32
 C      -3.406946    -3.414582     0.606663     117.51
 O      -3.939794    -4.717080     0.073270     173.33
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 H      -3.043284    -5.158137    -0.414865      25.23
 H      -4.265139    -3.111947     1.409640      24.97
 H      -2.692501    -3.358446     1.462158      27.09
 C       1.300321    -2.105356    -0.051416      49.41
 H       2.004657    -2.912721    -0.365295      24.47
 C       0.831822     0.078744     0.815810      56.10
 H       1.275908     1.014517     1.081130      20.85
 C      -0.574171     0.073848     0.617241      -1.43
 O      -1.383999     1.034323     1.347941     170.31
 C      -0.912374     2.056935     2.292373     110.49
 H      -1.462575     3.140628     2.083688      23.59
 H      -1.542149     1.793055     3.114314      27.14
 H       0.001505     1.952653     2.833294      26.55
 C      -1.005923    -1.197554     0.052116      21.16
 O      -2.385926    -1.173174     0.080168     173.68
 C      -0.094773    -2.212472    -0.162972      77.30
 H      -0.857500    -2.946162    -0.779223      21.72
 C       1.839554    -0.945690     0.347530      24.98
 C       3.227000    -0.325957     0.283756      98.41
 H       3.498147    -0.750968    -0.578958      27.44
 O       3.355338     1.133727     0.253265     192.79
 H       3.195216     1.581011     1.187218      23.92
 C       4.102757    -0.979239     1.411799      88.15
 H       3.707471    -0.432923     2.310497      25.41
 O       3.793866    -2.495270     1.492849     262.96
 H       4.130953    -2.680251     2.386389      28.76
 C       5.640323    -0.761348     1.313306      84.58
 O       6.220987     0.394415     1.842091     281.25
 H       6.147098     0.274322     2.797231      30.90
 H       5.841041    -0.633833     0.165638      28.67
 H       6.179503    -1.725718     1.714822      28.73
55
name= lig-ACN-Water-frame_1016
 C      -4.185120    -1.364048    -3.607034      78.33
 H      -4.101417    -2.398576    -3.869583      26.54
 C      -3.893579     0.523614    -2.092743      10.41
 H      -3.813879     0.909148    -0.924362      28.60
 C      -3.442130     1.329389    -3.203198      26.32
 O      -3.300250     2.732565    -3.268173     213.67
 C      -3.895836     3.456494    -2.186957     102.75
 H      -3.691947     4.524744    -2.394455      25.91
 H      -3.840861     3.415557    -0.989703      23.04
 H      -5.249008     3.383038    -2.171094      23.57
 C      -3.714027     0.825392    -4.482419      20.95
 O      -3.548730     1.714051    -5.519017     150.69
 H      -3.352770     2.680457    -5.290783      24.44
 C      -4.004531    -0.555836    -4.683118      69.74
 H      -4.100403    -1.158421    -5.670180      18.29
 C      -4.265559    -0.813685    -2.286687      14.20
 C      -4.621305    -1.760782    -1.016508      89.75
 H      -5.054574    -2.671442    -1.515684      24.12
 O      -5.692020    -1.310567    -0.197652     129.18
 H      -5.362432    -1.150107     0.681391      30.07
 C      -3.220314    -2.202037    -0.417452      84.71
 H      -2.787912    -2.514949    -1.356654      31.72
 C      -3.393916    -3.416165     0.736128     101.00
 O      -3.940405    -4.706068     0.042852     110.11
 H      -3.123010    -5.284734    -0.258556      27.13
 H      -4.241272    -3.020479     1.433952      24.82
 H      -2.446505    -3.841430     0.977718      24.97
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 C       1.271824    -2.065407    -0.107944      28.96
 H       1.907443    -2.956526    -0.465869      22.32
 C       0.926109     0.275542     0.691428      72.75
 H       1.089320     1.215941     1.279198      22.58
 C      -0.408939     0.009004     0.711808      27.16
 O      -1.315293     0.900439     1.193324     149.68
 C      -0.931104     2.008988     2.345332      94.92
 H      -0.856643     3.057991     1.747632      25.09
 H      -1.539584     1.831993     3.235780      26.13
 H       0.147635     1.922484     2.345288      25.29
 C      -1.069306    -1.170369     0.282287      29.19
 O      -2.451381    -1.068942     0.081508     149.53
 C      -0.210289    -2.262933    -0.045545      73.92
 H      -0.226922    -3.399952    -0.437259      22.01
 C       1.811661    -0.753670     0.318891      19.95
 C       3.318292    -0.472503     0.272969      94.24
 H       3.908617    -0.684792    -0.493257      28.76
 O       3.298589     1.131965     0.183334     146.16
 H       3.289814     1.489316     1.173337      22.81
 C       4.043104    -0.975308     1.537562      97.03
 H       3.777740    -0.645448     2.568178      24.10
 O       3.844746    -2.414795     1.503761     225.44
 H       4.252501    -2.983619     2.364954      26.45
 C       5.614301    -0.819921     1.360369      67.89
 O       6.211851     0.402394     1.889910     297.51
 H       6.221912     0.207999     2.813879      29.32
 H       5.962730    -0.967093     0.192839      28.49
 H       6.010348    -1.737858     1.883229      29.01
55
name= lig-ACN-Water-frame_1017
 C      -4.191004    -1.458178    -3.583307      32.50
 H      -4.539208    -2.456238    -3.616100      20.28
 C      -3.828144     0.517668    -2.129268      54.06
 H      -4.053317     1.087192    -1.079634      22.43
 C      -3.564496     1.333911    -3.207762       1.26
 O      -3.340058     2.789676    -3.142682     210.00
 C      -4.031367     3.557097    -2.113532      94.35
 H      -3.910002     4.658705    -2.259456      25.54
 H      -3.492763     3.033971    -1.251696      24.85
 H      -5.235476     3.145739    -2.360474      23.18
 C      -3.691206     0.781523    -4.570082      -6.10
 O      -3.535919     1.716411    -5.609460     142.07
 H      -3.471018     2.550423    -5.019454      19.00
 C      -4.119314    -0.577057    -4.798336      53.37
 H      -4.102669    -0.833936    -5.834725      26.65
 C      -4.147687    -0.898250    -2.257025      17.85
 C      -4.562237    -1.780085    -1.014285      93.42
 H      -4.989364    -2.741804    -1.352384      27.37
 O      -5.605116    -1.204712    -0.077627     161.19
 H      -5.215636    -0.844210     0.713099      27.54
 C      -3.247265    -2.235205    -0.410794      85.21
 H      -2.586015    -2.798899    -1.061520      28.29
 C      -3.383676    -3.466872     0.660897     122.47
 O      -3.929234    -4.577254     0.054716     246.32
 H      -3.280344    -4.881661    -0.523967      33.48
 H      -3.803134    -3.428594     1.706170      25.51
 H      -2.399402    -3.443239     1.080720      28.28
 C       1.129007    -1.869560    -0.057960      62.42
 H       1.901463    -2.685227    -0.073894      24.45
 C       1.013505     0.402718     0.645917      27.69
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 H       1.740973     1.313089     0.818474      15.09
 C      -0.397489    -0.020597     0.872839      -4.57
 O      -1.355905     0.961815     1.187472     193.30
 C      -0.855931     1.848169     2.163160     116.21
 H      -1.259270     2.881831     1.731986      24.28
 H      -1.551055     1.856545     3.074851      26.49
 H       0.098143     1.635554     2.749146      25.14
 C      -1.027210    -1.255872     0.412154     -15.10
 O      -2.567303    -1.016441     0.135926      76.28
 C      -0.169848    -2.318382    -0.003698      71.32
 H      -0.766092    -3.254161     0.049031      20.72
 C       1.806006    -0.709472     0.167851      20.58
 C       3.317694    -0.377206     0.294383      91.21
 H       3.681771    -0.836197    -0.513876      28.15
 O       3.350954     1.006782     0.114472     187.34
 H       3.583183     1.534516     0.919971      26.82
 C       4.147065    -1.028111     1.666598      85.07
 H       3.644458    -0.405563     2.424857      26.05
 O       3.851256    -2.386380     1.485526     263.65
 H       4.110926    -2.868436     2.412862      26.65
 C       5.623118    -0.889707     1.431161      86.97
 O       6.206197     0.410215     1.885393     270.65
 H       6.210220     0.344675     2.827723      31.12
 H       5.825720    -1.108702     0.221446      26.68
 H       6.181649    -1.644482     2.030041      28.48
55
name= lig-ACN-Water-frame_1018
 C      -4.284715    -1.428985    -3.597092      54.90
 H      -4.764221    -2.356483    -3.795193      22.25
 C      -3.837998     0.477779    -2.125568      44.59
 H      -3.894438     0.907155    -1.047528      21.49
 C      -3.738422     1.361622    -3.273071     -19.72
 O      -3.329407     2.722228    -3.134421     148.57
 C      -4.187035     3.522080    -2.015471      92.10
 H      -3.888953     4.536380    -2.409026      26.48
 H      -3.828034     3.522730    -0.960000      26.54
 H      -5.379972     3.549241    -1.628962      23.96
 C      -3.694380     0.806853    -4.595957      21.19
 O      -3.541926     1.674242    -5.655872     159.89
 H      -3.451539     2.606344    -5.423356      22.09
 C      -4.090509    -0.553322    -4.740050      46.51
 H      -4.334304    -0.955195    -5.617622      30.26
 C      -4.108771    -0.900411    -2.291489      24.67
 C      -4.476070    -1.771405    -1.068242      70.83
 H      -5.029700    -2.616629    -1.470457      27.51
 O      -5.445985    -1.104473    -0.002520     158.89
 H      -4.743736    -0.573909     0.579004      24.33
 C      -3.224727    -2.277648    -0.234037      98.68
 H      -2.698404    -2.513245    -1.148677      30.02
 C      -3.286604    -3.361028     0.720657     132.81
 O      -3.917315    -4.534452     0.014165     191.05
 H      -3.449346    -4.706826    -0.842082      30.90
 H      -4.054509    -2.991549     1.395170      26.90
 H      -2.372533    -3.791315     0.955314      27.24
 C       1.218356    -1.982892    -0.007095       0.86
 H       1.825048    -2.848464    -0.177660      25.01
 C       0.855100     0.336084     0.637076      68.57
 H       0.838601     1.508598     0.637050      23.58
 C      -0.442897     0.053778     0.861605      17.94
 O      -1.384282     0.958884     1.176132     207.43
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 C      -0.922701     1.905054     2.176027     101.67
 H      -0.570066     2.937066     1.851967      25.50
 H      -1.625756     1.724081     3.056599      24.89
 H       0.196266     1.475806     2.327102      24.10
 C      -1.113528    -1.146660     0.470284      18.38
 O      -2.486689    -1.113035     0.256138     138.12
 C      -0.262287    -2.231689     0.106181      56.89
 H      -0.313627    -3.198643    -0.247829      25.00
 C       1.765384    -0.593772     0.177162      25.45
 C       3.296601    -0.459821     0.286508     104.41
 H       3.853412    -0.906408    -0.413714      30.62
 O       3.582992     1.010073     0.041249     197.39
 H       3.651821     1.372984     0.919892      28.15
 C       4.094598    -0.946056     1.530880      97.88
 H       3.937295    -0.744479     2.592676      25.47
 O       3.811995    -2.452918     1.535963     295.42
 H       3.878663    -2.812823     2.373757      31.50
 C       5.737910    -0.884378     1.568983      86.57
 O       6.187045     0.407936     1.827049     242.41
 H       5.951228     0.493808     2.796458      28.22
 H       6.122654    -0.989382     0.358832      26.66
 H       6.111205    -1.747119     2.097464      31.05
55
name= lig-ACN-Water-frame_1019
 C      -4.404283    -1.316197    -3.617464      60.99
 H      -4.590613    -2.372486    -3.851653      32.45
 C      -3.881739     0.483292    -2.167863      68.82
 H      -3.527249     0.861834    -1.230568      29.96
 C      -3.773704     1.345492    -3.221376      36.81
 O      -3.496033     2.654916    -3.018410     215.47
 C      -4.199712     3.562538    -1.956601     102.07
 H      -4.205302     4.611448    -2.419042      26.19
 H      -3.672035     3.360485    -1.084670      27.03
 H      -5.149469     2.961518    -2.286446      24.19
 C      -3.791698     0.869971    -4.543029      28.22
 O      -3.555745     1.586526    -5.738546     177.88
 H      -3.354823     2.515319    -5.464163      25.85
 C      -4.044929    -0.524019    -4.700144      21.26
 H      -4.196722    -0.881028    -5.631055      15.84
 C      -4.166047    -0.884969    -2.283735       0.63
 C      -4.441239    -1.690948    -0.933978     106.26
 H      -5.017119    -2.579960    -1.183444      26.78
 O      -5.208853    -1.039895    -0.044157     244.08
 H      -4.822264    -0.420963     0.685530      22.70
 C      -3.046158    -2.224996    -0.371017      80.51
 H      -2.329107    -2.738141    -1.007761      29.41
 C      -3.326398    -3.403747     0.782923     107.88
 O      -3.964045    -4.488187     0.003668     150.51
 H      -3.087769    -4.811213    -0.601868      25.14
 H      -3.920451    -3.168197     1.608879      27.99
 H      -2.457640    -3.520132     1.380250      28.12
 C       1.216206    -1.976188     0.101324      92.82
 H       1.792123    -2.750757    -0.246601      27.40
 C       0.752894     0.333944     0.574345      35.88
 H       1.245153     1.370230     0.643061      24.29
 C      -0.675171     0.052409     0.724207       5.40
 O      -1.511666     1.077845     1.168057     141.05
 C      -0.881214     2.014858     2.315698      73.49
 H      -0.899779     2.927868     1.721586      25.38
 H      -1.620280     2.340364     3.173755      25.57
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 H       0.049516     1.503214     2.945488      24.86
 C      -1.078418    -1.207945     0.420829      19.16
 O      -2.469390    -1.193975     0.451024     169.43
 C      -0.137154    -2.148981     0.132381     112.70
 H      -0.673442    -2.861722    -0.241425      31.74
 C       1.745101    -0.734597     0.324708      -0.77
 C       3.348658    -0.451009     0.211486      77.23
 H       3.571564    -0.941309    -0.666906      27.66
 O       3.864464     0.999213     0.033434     217.54
 H       3.500945     1.622264     0.722095      27.66
 C       4.101246    -1.086597     1.513094      81.93
 H       3.569012    -0.356012     2.180806      25.91
 O       3.771981    -2.484633     1.555407     289.61
 H       3.873136    -2.740482     2.478051      29.40
 C       5.681728    -0.899962     1.472707      90.50
 O       6.202842     0.462950     1.850990     205.95
 H       6.003105     0.673355     2.897398      24.61
 H       6.356985    -1.424481     0.582784      26.98
 H       5.971418    -1.452231     2.355699      30.17
55
name= lig-ACN-Water-frame_1020
 C      -4.436050    -1.345426    -3.563755      30.83
 H      -4.656478    -2.455694    -3.677354      24.87
 C      -3.872556     0.477433    -2.073536      59.15
 H      -3.712648     0.878394    -1.166919      23.76
 C      -3.785826     1.386411    -3.187777      -8.83
 O      -3.551485     2.755364    -2.970958     243.08
 C      -4.257695     3.421452    -2.027268     134.79
 H      -4.221832     4.525352    -2.295598      26.90
 H      -3.820882     3.412185    -1.087959      29.04
 H      -5.332197     3.271117    -1.526953      26.06
 C      -3.888697     0.884909    -4.568547      23.70
 O      -3.586569     1.525189    -5.743977     128.19
 H      -3.253586     2.482761    -5.547358      22.76
 C      -4.092593    -0.475872    -4.751302      20.12
 H      -3.788914    -0.795238    -5.742099      24.65
 C      -4.308169    -0.869488    -2.235786      16.67
 C      -4.249544    -1.713595    -0.982529      92.76
 H      -4.810702    -2.630672    -1.192100      27.57
 O      -5.102014    -0.913791     0.016825     218.58
 H      -4.509106    -0.523535     0.611838      28.00
 C      -3.036031    -2.311406    -0.263109      89.12
 H      -2.380587    -2.518956    -1.133866      28.69
 C      -3.425710    -3.394638     0.721173     129.10
 O      -3.941230    -4.492605     0.040167     200.92
 H      -3.298261    -5.238209    -0.183936      27.69
 H      -4.169151    -3.023911     1.293010      28.17
 H      -2.536504    -3.790821     1.109389      27.32
 C       1.267163    -2.008057     0.159787       7.22
 H       1.949386    -2.826643     0.031247      23.49
 C       0.805822     0.329849     0.543056      68.07
 H       1.210806     1.317360     0.803264      25.28
 C      -0.597877     0.283169     0.679304       0.58
 O      -1.609890     1.240026     1.279750     149.82
 C      -0.956762     2.121536     2.330650      86.25
 H      -0.395643     2.951242     1.943237      26.69
 H      -1.995251     2.248142     2.859781      23.74
 H      -0.000919     1.630586     2.996691      24.82
 C      -1.087438    -1.090737     0.442828     -17.72
 O      -2.474861    -1.306565     0.576817     136.36
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 C      -0.171882    -2.292565     0.055371      45.13
 H      -0.251694    -3.274948     0.003734      24.25
 C       1.768208    -0.653129     0.473868      31.62
 C       3.370535    -0.404910     0.148146      92.04
 H       3.596369    -0.794463    -0.827208      26.86
 O       4.013815     0.861964     0.042107     223.84
 H       3.746154     1.449213     0.866104      25.58
 C       4.097688    -1.085979     1.343184      94.34
 H       3.806115    -0.670415     2.376024      23.56
 O       3.734482    -2.496604     1.594703     226.50
 H       4.122750    -2.935871     2.533647      25.74
 C       5.603665    -0.904445     1.593912      88.15
 O       6.199141     0.467289     1.804305     206.19
 H       6.246831     0.414789     2.843497      25.40
 H       6.060612    -1.250825     0.478675      28.49
 H       5.895643    -1.588100     2.362304      32.24
55
name= lig-ACN-Water-frame_1021
 C      -4.383213    -1.349266    -3.577625      71.85
 H      -4.633989    -2.449750    -3.839580      20.48
 C      -3.916740     0.556442    -2.045000      70.56
 H      -3.981317     0.873106    -1.106471      23.58
 C      -3.826603     1.399138    -3.182601     -15.33
 O      -3.559670     2.772019    -3.090298     164.98
 C      -4.351426     3.474979    -1.837207      88.25
 H      -4.403919     4.496611    -2.292287      26.37
 H      -3.746148     3.393600    -1.017198      28.41
 H      -5.417911     2.978745    -1.925100      26.64
 C      -3.912932     0.856529    -4.491710      -4.14
 O      -3.621743     1.557223    -5.709726     135.26
 H      -3.317979     2.478133    -5.637371      22.69
 C      -4.201533    -0.571151    -4.643172      25.26
 H      -4.144810    -1.219671    -5.612178      29.45
 C      -4.248975    -0.803813    -2.259133      12.95
 C      -4.328557    -1.729571    -0.998666      80.14
 H      -4.982842    -2.588850    -1.215860      28.20
 O      -5.011366    -0.860911     0.060239     207.60
 H      -4.419609    -0.527687     0.796457      26.26
 C      -3.045353    -2.300781    -0.252477      82.16
 H      -2.235184    -2.832423    -0.829656      26.69
 C      -3.475886    -3.439561     0.687534     116.57
 O      -4.044130    -4.660523     0.033355     233.82
 H      -3.264191    -5.076375    -0.142667      33.26
 H      -4.178566    -3.094232     1.297162      29.30
 H      -2.757147    -3.512736     1.473067      28.76
 C       1.235555    -1.973649     0.219908      73.84
 H       1.944333    -2.829897     0.392433      25.05
 C       0.902070     0.569957     0.665591      35.93
 H       1.234212     1.559500     0.685361      23.38
 C      -0.588925     0.293771     0.710750      14.15
 O      -1.472988     1.295787     1.289953     208.92
 C      -1.069190     2.190198     2.309561     102.70
 H      -0.555244     3.057995     1.928589      27.01
 H      -1.842228     2.776216     2.999194      25.45
 H      -0.686949     1.370573     3.126240      24.98
 C      -1.086819    -0.979851     0.442446     -13.19
 O      -2.375384    -1.358511     0.700084     162.42
 C      -0.072803    -2.224699     0.132379      38.46
 H      -0.643620    -3.092528     0.106560      24.19
 C       1.798998    -0.602673     0.378183       0.56
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 C       3.349848    -0.509061     0.199196      93.01
 H       3.587678    -1.138203    -0.696169      29.69
 O       4.009174     0.792561     0.070367     156.99
 H       4.288311     1.131117     0.958403      29.45
 C       4.053882    -1.058058     1.465837      77.39
 H       3.425365    -0.358809     2.160423      26.94
 O       3.721404    -2.532475     1.556498     203.52
 H       4.260129    -2.646031     2.503884      26.03
 C       5.640745    -0.939734     1.556933      94.50
 O       6.150322     0.372491     1.817273     183.15
 H       6.359250     0.584277     2.677827      28.87
 H       6.277687    -1.260545     0.515995      27.01
 H       5.996573    -1.634165     2.314453      31.63
55
name= lig-ACN-Water-frame_1022
 C      -4.334008    -1.395016    -3.442431      17.52
 H      -4.480479    -2.524216    -3.447889      27.93
 C      -4.041622     0.602058    -2.101737      52.72
 H      -3.888716     1.076263    -1.147177      31.46
 C      -3.837675     1.433134    -3.197612       5.76
 O      -3.626675     2.816516    -3.136135     170.84
 C      -4.354787     3.496809    -1.869781      94.39
 H      -4.706585     4.553564    -1.911457      25.23
 H      -3.847261     3.325876    -0.936788      26.76
 H      -5.223185     2.826304    -1.710913      24.39
 C      -3.878358     0.777449    -4.519183      15.63
 O      -3.691334     1.565936    -5.615998     156.20
 H      -3.574485     2.410887    -5.171532      23.81
 C      -4.249599    -0.535486    -4.645732      40.22
 H      -4.676610    -0.710356    -5.783174      22.19
 C      -4.108643    -0.841001    -2.196447      14.63
 C      -4.424521    -1.585345    -0.904958      79.96
 H      -5.083879    -2.462252    -1.107900      24.87
 O      -4.982193    -0.856186     0.059056     264.32
 H      -4.374891    -0.834929     0.956632      21.59
 C      -3.047154    -2.340335    -0.280502      42.21
 H      -2.333525    -2.536057    -1.145476      26.05
 C      -3.665258    -3.528157     0.794233     100.68
 O      -4.061701    -4.780700     0.053434     147.83
 H      -3.452923    -5.066760    -0.721800      28.86
 H      -4.505482    -3.256087     1.228315      27.99
 H      -2.821948    -3.894357     1.325827      26.65
 C       1.287873    -1.787026     0.305044      19.72
 H       1.974948    -2.714741     0.142497      24.56
 C       0.962088     0.584371     0.692141      72.32
 H       1.475902     1.460483     0.780116      25.71
 C      -0.447081     0.351392     0.868538      -4.63
 O      -1.399182     1.277837     1.152556     158.25
 C      -1.106329     2.234093     2.388184      81.96
 H      -0.290255     2.810294     1.981199      28.10
 H      -2.155500     2.622465     2.225667      24.38
 H      -0.573940     2.007297     3.452441      25.37
 C      -0.954038    -0.961807     0.433663      15.07
 O      -2.333037    -1.383852     0.747261     125.42
 C      -0.141009    -1.952491     0.316931      52.73
 H      -0.439335    -3.034003     0.149882      24.05
 C       1.750571    -0.487563     0.266603      20.47
 C       3.349619    -0.583959     0.299154      83.88
 H       3.742556    -1.222202    -0.623815      29.51
 O       3.922521     0.756122     0.050625     161.23
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 H       4.123954     1.100685     0.913615      30.04
 C       4.009621    -1.131794     1.599918      96.04
 H       3.792057    -0.673393     2.659200      25.85
 O       3.774246    -2.495160     1.577138     313.56
 H       3.806148    -3.040820     2.312071      32.33
 C       5.650329    -1.023275     1.518061      72.56
 O       6.133174     0.346226     1.871560     196.44
 H       5.759696     0.254378     2.765930      29.11
 H       5.933297    -1.489670     0.375604      26.36
 H       5.979030    -1.709338     2.323981      30.24
55
name= lig-ACN-Water-frame_1023
 C      -4.250590    -1.380793    -3.431436      48.81
 H      -4.481589    -2.433527    -3.553476      19.26
 C      -4.053607     0.619341    -2.085841      73.49
 H      -4.042784     1.094020    -1.016771      28.45
 C      -3.841106     1.402566    -3.231388       7.27
 O      -3.759247     2.902121    -3.117887     180.44
 C      -4.334083     3.390801    -1.957526     121.35
 H      -4.367674     4.400733    -2.408399      25.39
 H      -3.459512     3.510882    -1.247084      26.17
 H      -5.257119     3.049341    -1.586164      26.25
 C      -3.870557     0.806551    -4.449569       8.39
 O      -3.757385     1.628924    -5.552609     132.46
 H      -3.733718     2.640150    -5.404870      20.82
 C      -4.309356    -0.592195    -4.568000      10.36
 H      -4.669186    -1.080045    -5.668132      30.91
 C      -4.091822    -0.755286    -2.118256      17.51
 C      -4.267969    -1.616264    -0.826455      72.25
 H      -4.980187    -2.373617    -1.218688      29.18
 O      -5.073866    -0.754280     0.164495     177.21
 H      -4.491613    -0.579188     1.088572      22.45
 C      -3.196149    -2.354206    -0.133173      69.68
 H      -2.567132    -2.866335    -0.924493      29.69
 C      -3.703353    -3.638552     0.706021     122.98
 O      -4.081257    -4.846307     0.036061     157.62
 H      -3.410651    -4.768306    -0.803505      29.54
 H      -4.491169    -3.255896     1.209877      29.47
 H      -3.093041    -3.748738     1.598444      28.38
 C       1.276207    -1.689744     0.237326      67.79
 H       1.979045    -2.541459    -0.098427      26.06
 C       1.054066     0.590247     0.667627      70.84
 H       1.250840     1.531423     1.093356      27.38
 C      -0.378203     0.353739     0.901473      20.71
 O      -1.315952     1.317582     1.171947     215.03
 C      -1.134479     2.304186     2.262546     109.62
 H      -0.360125     3.123707     2.171293      26.60
 H      -2.026837     2.982399     2.443022      26.16
 H      -1.391690     1.550414     3.093658      24.81
 C      -1.031926    -0.851513     0.615651       1.45
 O      -2.324774    -1.386194     0.668084     140.90
 C      -0.013928    -1.995370     0.421489      30.43
 H      -0.380379    -3.119796     0.351396      25.96
 C       1.919586    -0.452171     0.342122      47.49
 C       3.336934    -0.445056     0.416635      86.55
 H       3.734584    -1.259333    -0.413333      26.54
 O       3.853851     0.760974     0.030099     192.29
 H       3.593908     1.486203     0.694099      26.54
 C       4.126780    -1.189297     1.707694      85.75
 H       3.692685    -0.765282     2.687150      26.15
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 O       3.759791    -2.624989     1.580222     272.78
 H       3.855025    -2.772326     2.494202      30.26
 C       5.553821    -1.074463     1.555879      86.00
 O       6.092298     0.245458     1.947026     190.28
 H       5.857061     0.722051     2.879797      25.85
 H       5.993365    -1.028850     0.336432      23.53
 H       6.120965    -1.931300     2.012339      28.46
55
name= lig-ACN-Water-frame_1024
 C      -4.205323    -1.341785    -3.336972      69.76
 H      -4.372210    -2.363347    -3.437796      21.94
 C      -3.956502     0.677681    -1.972181      72.23
 H      -4.204958     1.211049    -0.911647      22.16
 C      -3.864391     1.452570    -3.106360       1.19
 O      -3.889076     2.745611    -3.246595     201.85
 C      -4.238149     3.543772    -1.991372     117.63
 H      -4.615661     4.543842    -2.135591      25.73
 H      -3.622570     3.302580    -1.049298      25.81
 H      -5.078917     3.032867    -1.679119      28.08
 C      -3.970917     0.833146    -4.480534       4.39
 O      -3.823988     1.662269    -5.608574     151.10
 H      -3.780786     2.545379    -5.130233      19.82
 C      -4.242764    -0.525790    -4.517738      53.20
 H      -4.208140    -1.232779    -5.521811      29.38
 C      -4.094151    -0.769435    -2.086308      32.41
 C      -4.320106    -1.534393    -0.736475      67.12
 H      -5.026870    -2.376196    -0.910287      29.44
 O      -5.146363    -0.707920     0.225474     212.75
 H      -4.545993    -0.498022     1.071647      24.71
 C      -3.117928    -2.430396    -0.051999      74.78
 H      -2.403411    -2.833094    -0.787126      29.20
 C      -3.762441    -3.560288     0.812150     101.09
 O      -4.039370    -4.826141    -0.064765     105.63
 H      -3.310115    -5.269793    -0.501263      31.18
 H      -4.744922    -3.502965     1.165276      28.08
 H      -2.941930    -3.878202     1.455580      27.77
 C       1.378988    -1.752388     0.099553      49.12
 H       2.022004    -2.643954    -0.005887      23.39
 C       1.011547     0.667819     0.780802      44.98
 H       1.559364     1.636501     0.896784      22.46
 C      -0.455928     0.351649     0.859588     -12.05
 O      -1.284093     1.465793     1.140354     203.14
 C      -1.234527     2.352758     2.235380     105.00
 H      -0.157974     2.609409     2.341212      25.98
 H      -2.051744     3.016722     1.963105      25.38
 H      -1.176708     1.898342     3.335792      26.03
 C      -0.972068    -1.119659     0.729048      -0.10
 O      -2.404259    -1.304870     0.659922     141.77
 C       0.010424    -2.038781     0.446751      56.51
 H      -0.526492    -3.106632     0.340700      25.04
 C       1.902071    -0.472187     0.539080       9.19
 C       3.487169    -0.451818     0.510068      74.24
 H       3.737632    -1.091624    -0.529853      23.35
 O       3.896129     0.948147     0.020836     149.44
 H       3.300650     1.587854     0.530105      26.10
 C       4.037765    -1.206793     1.700670      86.59
 H       3.708838    -0.741073     2.674825      24.70
 O       3.731304    -2.721245     1.641203     207.99
 H       4.128265    -3.349429     2.424768      26.04
 C       5.653430    -1.020585     1.585611      78.82
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 O       6.098015     0.188605     2.039183     236.72
 H       5.942332     0.062613     3.099478      24.29
 H       5.711645    -1.107112     0.302622      26.09
 H       6.176408    -1.942215     2.049058      28.57
55
name= lig-ACN-Water-frame_1025
 C      -4.192554    -1.309412    -3.246194      35.78
 H      -4.207199    -2.339031    -3.308191      29.47
 C      -3.889878     0.648970    -1.878702      53.97
 H      -3.812123     1.219230    -0.849907      22.31
 C      -3.952607     1.347695    -3.158866      20.49
 O      -3.973908     2.841255    -3.291018     144.97
 C      -4.258885     3.588497    -2.013660     115.61
 H      -4.128894     4.607839    -2.372884      26.66
 H      -3.225718     3.520121    -1.426811      26.00
 H      -5.111586     3.308327    -1.574912      29.32
 C      -4.044940     0.858057    -4.433581      31.01
 O      -3.913452     1.652078    -5.592192     174.74
 H      -3.665112     2.541827    -5.414645      27.00
 C      -4.059923    -0.540855    -4.507624       5.94
 H      -4.043165    -0.852834    -5.645132      17.23
 C      -4.086992    -0.714474    -1.903538       7.45
 C      -4.478075    -1.548660    -0.681309      76.77
 H      -5.201967    -2.306037    -1.093829      24.60
 O      -5.130270    -0.714232     0.263427     267.70
 H      -4.644972    -0.631652     1.107125      26.87
 C      -3.099255    -2.288403    -0.029800      64.44
 H      -2.542430    -2.677868    -0.860392      28.26
 C      -3.721098    -3.612859     0.856250     105.71
 O      -3.973671    -4.745242    -0.126514     181.77
 H      -3.082452    -4.980743    -0.045493      31.01
 H      -4.559756    -3.069767     1.348472      27.40
 H      -3.233106    -3.969207     1.779590      28.62
 C       1.397101    -1.795493     0.203614      41.73
 H       2.142527    -2.434819    -0.168293      24.85
 C       0.920086     0.482057     0.911224      56.29
 H       1.044195     1.642948     0.883868      20.31
 C      -0.473157     0.330623     0.899987      16.76
 O      -1.358480     1.438579     0.966519     138.79
 C      -1.174583     2.409387     2.323406      91.24
 H      -0.216198     3.016381     2.331185      23.82
 H      -1.725206     3.284639     2.028709      26.70
 H      -1.901646     2.053987     3.076333      24.90
 C      -0.984243    -1.010865     0.790159     -18.93
 O      -2.381758    -1.237043     0.718340     148.35
 C       0.074294    -2.240515     0.343228      28.95
 H      -0.014454    -3.380924     0.002085      22.45
 C       1.844245    -0.532198     0.600365      40.69
 C       3.389129    -0.407501     0.431260      43.72
 H       3.970739    -1.015794    -0.508466      23.65
 O       3.966187     1.045436     0.094432     180.26
 H       3.753774     1.641945     0.829305      27.13
 C       4.132178    -1.254696     1.738778      73.67
 H       3.738010    -0.925776     2.706241      24.18
 O       3.692367    -2.692357     1.646756     172.75
 H       4.435482    -2.881975     2.440310      25.08
 C       5.621345    -1.120165     1.562876      76.60
 O       6.155839     0.180069     2.189640     215.90
 H       6.182410     0.260214     3.209985      25.79
 H       6.240586    -1.149513     0.434280      25.90
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 H       6.141588    -1.958829     2.202004      27.72
55
name= lig-ACN-Water-frame_1026
 C      -4.119268    -1.267181    -3.221949      71.49
 H      -4.301253    -2.304443    -3.332318      29.92
 C      -3.858573     0.742372    -1.919538      66.48
 H      -3.497447     1.270804    -1.035378      23.42
 C      -4.039486     1.528123    -3.080362     -23.99
 O      -4.076088     2.869527    -3.238578     211.36
 C      -4.146751     3.688093    -2.109826     129.53
 H      -4.176368     4.704062    -2.493028      27.81
 H      -3.355811     3.322056    -1.292036      25.67
 H      -4.976979     3.644218    -1.561363      30.74
 C      -4.003477     0.816640    -4.405203       4.40
 O      -4.019651     1.576760    -5.565616     139.86
 H      -3.644136     2.468185    -5.274514      21.02
 C      -3.918709    -0.623110    -4.412559      87.18
 H      -3.964463    -1.378320    -5.208501      21.45
 C      -4.133711    -0.713330    -1.927068      24.50
 C      -4.418828    -1.561539    -0.615478      78.81
 H      -5.097291    -2.459522    -0.821406      26.68
 O      -5.155564    -0.737958     0.339918     270.38
 H      -4.548074    -0.605333     1.082324      27.05
 C      -3.197561    -2.197172     0.008959      84.23
 H      -2.543526    -2.520753    -0.757041      30.28
 C      -3.656457    -3.503039     0.839412      94.91
 O      -3.870178    -4.585299    -0.057402     143.57
 H      -3.157870    -5.007397    -0.725407      26.68
 H      -4.801946    -3.542991     1.123651      23.59
 H      -2.919686    -3.781207     1.608800      26.81
 C       1.376813    -1.892750     0.344989      39.62
 H       1.947614    -2.531499    -0.211595      28.07
 C       0.873746     0.387809     0.993863      46.02
 H       1.494974     1.379468     1.292184      21.62
 C      -0.554816     0.178919     1.003726     -22.11
 O      -1.394941     1.415594     0.942840     100.41
 C      -1.206882     2.473514     2.166768     112.01
 H      -0.290535     2.230398     2.680541      26.43
 H      -1.756718     3.291518     1.847683      26.94
 H      -1.545871     1.808328     2.996485      27.27
 C      -0.913846    -1.197219     0.630690       0.64
 O      -2.335107    -1.209666     0.775884     144.41
 C      -0.029410    -2.118648     0.306973      81.74
 H      -0.604774    -3.044557    -0.050579      24.22
 C       1.873074    -0.521567     0.558873      17.07
 C       3.364327    -0.277537     0.457256      84.10
 H       3.401656    -0.905137    -0.651794      25.36
 O       3.958579     0.988286     0.271140     212.33
 H       4.215633     1.278280     1.171328      26.73
 C       4.155599    -1.182977     1.611439      86.99
 H       3.925821    -0.619229     2.513212      27.18
 O       3.730969    -2.568699     1.639376     288.77
 H       3.899455    -3.172170     2.376287      29.39
 C       5.734585    -1.135729     1.745578      84.31
 O       6.199007     0.102651     2.224020     236.34
 H       5.937457     0.126769     3.162461      28.84
 H       6.030832    -1.097597     0.512358      26.65
 H       6.114817    -2.163656     2.243597      28.37
55
name= lig-ACN-Water-frame_1027
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 C      -4.071292    -1.392812    -3.113720      27.18
 H      -4.324473    -2.478918    -3.125326      20.71
 C      -3.888646     0.801653    -1.904029      72.28
 H      -3.888645     1.207954    -0.992336      23.96
 C      -4.051349     1.491761    -3.119143      -2.36
 O      -4.159969     2.891530    -3.269258     156.69
 C      -4.090326     3.867851    -2.057536     109.25
 H      -3.756335     4.862828    -2.432597      26.63
 H      -3.256507     3.561868    -1.294543      26.22
 H      -4.959934     3.769901    -1.685297      30.17
 C      -3.941280     0.755859    -4.340009      18.11
 O      -4.090139     1.480669    -5.534241     150.18
 H      -3.904240     2.467002    -5.336845      20.24
 C      -3.852261    -0.609444    -4.360438      76.20
 H      -3.688398    -0.956810    -5.319036      29.59
 C      -4.134870    -0.599997    -1.925409      19.52
 C      -4.348862    -1.408061    -0.598057      86.81
 H      -4.978139    -2.290723    -1.000985      26.71
 O      -5.189064    -0.788568     0.413072     253.05
 H      -4.706827    -0.272426     1.185047      24.10
 C      -3.160750    -2.181059     0.048811      85.14
 H      -2.629741    -2.614004    -0.766522      30.32
 C      -3.589456    -3.367399     0.822631     115.00
 O      -3.787791    -4.536421    -0.062649     142.65
 H      -2.984570    -4.262185    -0.705221      28.19
 H      -4.347117    -3.099993     1.731066      23.97
 H      -2.710737    -3.496288     1.503699      26.35
 C       1.311156    -1.913483     0.304378      66.64
 H       1.920092    -2.768966     0.289859      25.03
 C       0.912267     0.402073     1.081233      63.26
 H       1.153774     1.469727     1.544988      19.15
 C      -0.459636     0.170591     1.018727      14.07
 O      -1.369552     1.308232     1.020006     235.27
 C      -1.243502     2.215230     2.012783     149.15
 H      -0.237871     2.625357     2.077102      26.37
 H      -1.349747     3.212464     1.631424      28.27
 H      -2.039353     2.293037     2.765583      27.13
 C      -1.068162    -1.013674     0.603020      14.37
 O      -2.389276    -1.284273     0.800281     175.34
 C      -0.097198    -2.102501     0.257737      38.21
 H      -0.317300    -3.151168    -0.029862      25.13
 C       1.782203    -0.642806     0.642515      21.75
 C       3.429448    -0.420739     0.447636      67.57
 H       3.887711    -0.736967    -0.670026      23.84
 O       3.930239     0.944201     0.485831     192.04
 H       3.915856     1.472759     1.414285      22.47
 C       4.161209    -1.070709     1.607354     100.17
 H       3.680480    -0.644034     2.457568      26.06
 O       3.728505    -2.453295     1.571824     298.63
 H       3.854724    -2.526408     2.444254      31.54
 C       5.744936    -1.163032     1.699088      80.45
 O       6.245943     0.050241     2.256579     216.25
 H       6.111605     0.255165     3.154006      30.23
 H       6.445149    -1.466322     0.697594      26.76
 H       6.025220    -1.991694     2.568003      28.17
55
name= lig-ACN-Water-frame_1028
 C      -4.009656    -1.350479    -3.117502      50.03
 H      -3.919150    -2.516207    -3.069576      30.34
 C      -4.033731     0.839239    -1.859249      78.32
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 H      -4.263093     1.434650    -1.066021      26.51
 C      -3.986668     1.521314    -3.083658       5.35
 O      -4.191958     2.978799    -3.278369     153.57
 C      -4.093999     3.887345    -2.080380     113.36
 H      -3.668629     4.763995    -2.640331      26.22
 H      -3.449889     3.278589    -1.371153      25.27
 H      -4.809426     4.301036    -1.587097      29.67
 C      -3.935999     0.795753    -4.302589      20.02
 O      -4.116983     1.370689    -5.524057     181.51
 H      -4.163108     2.307943    -5.412274      26.00
 C      -3.822797    -0.689656    -4.292397      50.16
 H      -3.678228    -1.152233    -5.169762      20.29
 C      -4.038201    -0.580919    -1.828626      25.03
 C      -4.395051    -1.303712    -0.609452      77.07
 H      -5.145131    -2.102278    -0.990757      20.25
 O      -5.228713    -0.837762     0.467127     237.19
 H      -4.740628    -0.039953     0.917720      25.44
 C      -3.132052    -2.114700    -0.098246      70.53
 H      -2.411989    -2.342569    -0.857997      28.28
 C      -3.421556    -3.330402     0.944347      91.15
 O      -3.747249    -4.429977    -0.035102     171.18
 H      -2.956161    -4.704499    -0.494518      30.92
 H      -4.514695    -3.078526     1.471567      22.33
 H      -2.544995    -3.710794     1.496373      25.28
 C       1.163756    -1.878390     0.264337      59.46
 H       1.873419    -2.734055     0.173457      25.16
 C       1.013624     0.358157     1.118949      86.33
 H       1.512665     1.396361     1.231486      17.94
 C      -0.427386     0.223540     0.957901      21.11
 O      -1.397902     1.080895     1.063782     199.07
 C      -1.229699     2.318856     1.899888     113.05
 H      -0.334959     2.122956     2.473333      27.16
 H      -1.664067     2.951886     1.217707      26.94
 H      -1.869565     2.071687     2.783991      26.43
 C      -1.020865    -1.046642     0.581771      -2.23
 O      -2.454485    -1.250225     0.895756     134.46
 C      -0.206870    -2.105940     0.233446      74.03
 H      -0.643952    -3.083170     0.117501      26.36
 C       1.896591    -0.662667     0.716532      25.82
 C       3.446338    -0.448885     0.509769      80.75
 H       3.704246    -1.100750    -0.499987      24.11
 O       3.876363     0.971194     0.582994     212.66
 H       3.495038     1.327567     1.497226      21.65
 C       4.198876    -1.088514     1.613441     113.56
 H       4.037226    -0.524845     2.489622      25.73
 O       3.709035    -2.422679     1.590796     242.84
 H       3.944368    -3.193849     2.278402      26.09
 C       5.679784    -1.156504     1.756197      78.69
 O       6.355007     0.082138     2.224807     196.62
 H       5.993997     0.250182     3.083770      32.53
 H       6.225168    -1.468403     0.716737      27.64
 H       5.732533    -2.142682     2.502283      27.47
55
name= lig-ACN-Water-frame_1029
 C      -3.837651    -1.223167    -2.960815      38.76
 H      -3.717418    -2.400158    -2.966478      29.10
 C      -4.201964     0.902895    -1.869368      66.07
 H      -4.448098     1.346839    -0.834048      29.44
 C      -3.971067     1.645905    -3.071059     -18.57
 O      -4.247101     2.961747    -3.246686     211.81
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 C      -4.050237     3.861230    -2.181171     132.99
 H      -3.359919     4.690364    -2.452146      27.69
 H      -3.568691     3.438582    -1.260051      26.78
 H      -4.960838     4.034803    -1.985634      29.49
 C      -3.926416     0.735733    -4.293821      11.84
 O      -4.115683     1.285022    -5.572061     157.61
 H      -4.173349     2.266943    -5.466991      28.30
 C      -3.817865    -0.626080    -4.269430     116.23
 H      -3.896406    -1.264999    -5.055149      24.80
 C      -4.040748    -0.516823    -1.837091      19.35
 C      -4.459633    -1.491583    -0.556813      67.78
 H      -5.062725    -2.386000    -0.968000      23.65
 O      -5.239197    -0.804163     0.491649     228.13
 H      -4.828597    -0.000612     0.769176      31.82
 C      -3.114940    -2.060646     0.020326      75.33
 H      -2.583458    -2.290053    -0.912388      34.73
 C      -3.308771    -3.325289     0.770445     120.41
 O      -3.757619    -4.412469     0.017340     195.66
 H      -3.028908    -5.006005    -0.104334      29.84
 H      -4.256397    -3.191333     1.616998      24.27
 H      -2.582211    -3.339757     1.605562      26.90
 C       1.243073    -1.897546     0.250672      50.44
 H       1.672060    -2.679902    -0.466417      27.24
 C       1.057855     0.371044     1.053319      70.87
 H       1.484315     1.365283     1.233610      21.49
 C      -0.333423     0.094852     0.892671       6.36
 O      -1.487373     1.030932     1.131731     151.86
 C      -1.276455     2.358492     1.864896     123.21
 H      -0.238162     2.613466     2.133795      28.44
 H      -1.240652     3.372904     1.532383      29.29
 H      -2.065987     2.355159     2.616062      28.97
 C      -1.038007    -1.098504     0.687851      28.72
 O      -2.365050    -1.088845     0.914021     123.73
 C      -0.248577    -2.145345     0.245721      42.36
 H      -0.617204    -3.106338    -0.081233      26.51
 C       1.854219    -0.737074     0.674351      28.36
 C       3.389941    -0.391353     0.615091      79.69
 H       3.724830    -0.603874    -0.532320      25.57
 O       3.755362     0.938781     0.504315     207.86
 H       4.142904     1.409255     1.354897      26.35
 C       4.177012    -1.165568     1.812154      96.16
 H       3.707116    -0.802264     2.668614      29.57
 O       3.641150    -2.536452     1.643372     233.76
 H       4.501816    -3.024231     2.159891      28.12
 C       5.764860    -1.123936     1.783412      90.08
 O       6.367535     0.053659     2.147007     165.33
 H       6.170267     0.410931     3.113683      26.73
 H       6.112990    -1.340021     0.667158      28.53
 H       6.320748    -1.927246     2.531733      28.24
55
name= lig-ACN-Water-frame_1030
 C      -3.649922    -1.201747    -2.921521      18.69
 H      -3.677232    -2.353083    -2.774452      20.28
 C      -4.310395     0.909805    -1.850488      83.53
 H      -4.689651     1.737843    -1.009268      21.86
 C      -4.062859     1.493482    -3.125576      27.70
 O      -4.240755     2.901271    -3.321093     168.26
 C      -4.085276     3.862778    -2.184107     128.40
 H      -3.607250     4.704884    -2.675256      27.61
 H      -3.738492     3.372671    -1.308625      27.03
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 H      -4.928233     4.391020    -1.956551      29.25
 C      -3.925877     0.846497    -4.297259      25.32
 O      -4.088480     1.251135    -5.618485     145.87
 H      -3.986993     2.269712    -5.706290      20.77
 C      -3.806926    -0.600696    -4.160100      20.97
 H      -3.779717    -0.978444    -5.168945      29.50
 C      -4.176839    -0.487601    -1.687457      -0.63
 C      -4.392221    -1.432026    -0.481946     100.03
 H      -4.979762    -2.354175    -0.789021      29.09
 O      -5.261175    -0.809368     0.467788     260.62
 H      -4.797198     0.051866     0.623598      30.58
 C      -3.078154    -1.979364     0.080725     100.41
 H      -2.339652    -2.217632    -0.724429      32.05
 C      -3.302186    -3.302251     0.864878     101.33
 O      -3.768617    -4.517840     0.044770     110.72
 H      -2.826629    -4.839980    -0.423960      26.48
 H      -4.131672    -2.996404     1.769041      25.56
 H      -2.331868    -3.740060     1.011354      26.16
 C       1.243277    -2.015032     0.126831      48.22
 H       2.126841    -2.615514    -0.322560      23.43
 C       0.927675     0.348753     0.934415      63.93
 H       1.299420     1.245849     1.312117      24.66
 C      -0.465307     0.241838     1.002607      12.77
 O      -1.435361     1.148911     1.207878     211.51
 C      -1.250439     2.395882     1.834686     115.07
 H      -0.291067     2.196945     2.332876      27.26
 H      -1.510259     2.779458     0.899316      26.41
 H      -1.899597     2.614104     2.669137      28.15
 C      -0.937356    -1.126526     0.793562     -11.17
 O      -2.403400    -1.008284     0.823777     122.11
 C      -0.068957    -2.228464     0.251483      68.82
 H      -0.421856    -3.165993    -0.260609      26.46
 C       1.842682    -0.722894     0.617442      14.64
 C       3.401332    -0.500923     0.681576      70.92
 H       3.906332    -1.318812    -0.046630      24.45
 O       3.652177     1.036984     0.439880     195.62
 H       3.944365     1.337749     1.293648      27.47
 C       4.018093    -1.240066     1.927948      88.73
 H       3.886320    -0.911649     2.906141      27.98
 O       3.696645    -2.664602     1.730197     265.63
 H       4.218597    -3.264339     2.316251      29.10
 C       5.800191    -1.196112     1.761218      64.28
 O       6.362346     0.173714     2.115228     137.58
 H       6.152289     0.131205     3.174637      26.70
 H       6.059396    -1.346409     0.687284      30.56
 H       6.156404    -2.194858     2.386904      28.99
55
name= lig-ACN-Water-frame_1031
 C      -3.697529    -1.165082    -2.809357      78.16
 H      -3.296404    -2.196916    -2.917683      26.69
 C      -4.406339     0.869301    -1.845984      77.75
 H      -4.917988     1.550361    -0.936138      22.35
 C      -4.244119     1.542397    -3.089177     -78.98
 O      -4.233246     2.879529    -3.359099     179.68
 C      -4.170778     3.870917    -2.258101     131.55
 H      -3.425714     4.497845    -2.641662      28.31
 H      -3.627268     3.490621    -1.440141      29.14
 H      -5.069056     4.187817    -1.954079      29.68
 C      -3.944187     0.748304    -4.350162       3.61
 O      -4.036943     1.270461    -5.655167     145.80
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 H      -3.763718     2.181646    -5.666115      20.33
 C      -3.701791    -0.556692    -4.120508      81.12
 H      -3.344380    -1.383590    -4.787642      31.36
 C      -4.167724    -0.533866    -1.733393      55.20
 C      -4.359821    -1.303198    -0.471548      99.78
 H      -4.888620    -2.199356    -0.871621      30.52
 O      -5.276151    -0.784932     0.493795     240.61
 H      -5.087547     0.153748     0.897925      27.19
 C      -3.046341    -2.012816     0.012963      76.27
 H      -2.568251    -2.354831    -0.969648      32.99
 C      -3.242465    -3.401046     0.955307      86.00
 O      -3.772084    -4.548458     0.088447     139.41
 H      -3.223867    -4.525348    -0.807510      29.17
 H      -3.931652    -3.618658     1.981086      23.00
 H      -2.283454    -3.427979     1.549552      26.08
 C       1.440053    -1.927399     0.084870      45.57
 H       1.883860    -2.952720    -0.065242      21.25
 C       0.899924     0.373581     0.906118      62.82
 H       1.424975     1.268263     0.957294      24.27
 C      -0.495899     0.152182     1.114806      18.30
 O      -1.458717     1.150100     1.294098     183.51
 C      -1.138909     2.506096     1.777332     129.93
 H      -0.194038     2.911733     2.174227      27.44
 H      -1.111390     3.483925     1.285050      28.25
 H      -1.987316     2.580502     2.429636      28.69
 C      -0.903128    -1.136997     0.774138      13.77
 O      -2.371039    -1.017901     0.784565      80.06
 C      -0.083476    -2.180858     0.275193      33.72
 H      -0.756973    -3.107699     0.044265      27.35
 C       1.796799    -0.704296     0.524878      33.96
 C       3.308819    -0.584456     0.745004      74.98
 H       3.802428    -0.856220    -0.286190      25.68
 O       3.591047     0.945951     0.435458     217.97
 H       3.535763     1.532324     1.189976      27.15
 C       4.153360    -1.318721     1.982646      92.95
 H       3.731291    -0.905680     2.861088      27.23
 O       3.747993    -2.748282     1.819537     321.94
 H       3.878181    -3.020551     2.660319      33.25
 C       5.620088    -1.159752     1.738679      97.69
 O       6.301403     0.160394     2.135439     226.68
 H       6.246343     0.342122     3.099612      28.98
 H       5.897004    -1.391975     0.744003      31.65
 H       6.212173    -1.843915     2.528797      27.92
55
name= lig-ACN-Water-frame_1032
 C      -3.729614    -1.218373    -2.871099      66.84
 H      -3.369973    -2.154610    -2.560387      29.65
 C      -4.544568     0.883072    -1.886461      85.55
 H      -4.780158     1.324444    -0.805044      26.96
 C      -4.351600     1.508536    -3.165656      14.57
 O      -4.247706     2.904584    -3.376280     174.89
 C      -4.177613     3.836432    -2.321711     140.25
 H      -4.027093     4.791560    -2.662625      28.69
 H      -3.748946     3.421179    -1.476173      29.44
 H      -5.169798     4.053358    -2.128561      28.05
 C      -4.020981     0.725265    -4.292251       9.94
 O      -3.951254     1.287491    -5.634884     146.09
 H      -3.648836     2.212431    -5.501603      24.93
 C      -3.510542    -0.668615    -4.125397      14.57
 H      -3.107632    -1.071714    -5.157851      17.54
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 C      -4.136824    -0.424259    -1.732263      -3.16
 C      -4.430600    -1.370248    -0.453933      76.20
 H      -5.123738    -2.151950    -0.772467      24.65
 O      -5.299261    -0.735934     0.558259     250.31
 H      -4.811976    -0.046875     1.037516      28.91
 C      -3.154906    -2.134648     0.113895      90.77
 H      -2.490529    -2.477704    -0.762617      29.26
 C      -3.233155    -3.472004     0.934478     118.68
 O      -3.721827    -4.508887     0.175204     216.44
 H      -3.278432    -4.576481    -0.615610      33.60
 H      -4.148279    -2.997983     1.571102      24.08
 H      -2.221777    -3.773639     1.297487      25.18
 C       1.219768    -1.964836     0.168078      68.88
 H       2.075736    -2.571307    -0.084091      24.93
 C       0.988970     0.400470     0.912886      72.07
 H       1.108338     1.467623     0.910455      23.88
 C      -0.333814     0.151091     1.121495      -4.13
 O      -1.425007     1.162011     1.365892     118.64
 C      -1.047131     2.684702     1.794515     109.39
 H      -0.145492     2.318295     2.291091      26.29
 H      -1.173763     3.042920     0.771364      27.61
 H      -1.734375     3.058128     2.554387      28.79
 C      -0.986864    -1.076047     0.728259      34.91
 O      -2.279860    -1.156135     0.739111     147.57
 C      -0.090758    -2.084628     0.281645      82.15
 H      -0.275843    -3.227807     0.038642      25.28
 C       1.835076    -0.701661     0.551139      19.19
 C       3.292440    -0.466205     0.660380      98.04
 H       3.738958    -1.160952    -0.238743      24.78
 O       3.597856     0.809328     0.487026     260.86
 H       3.565945     1.309032     1.428896      21.77
 C       4.049204    -1.289610     1.877742      94.96
 H       3.825140    -0.921324     2.886289      25.51
 O       3.778809    -2.723871     1.900096     269.42
 H       4.159903    -3.266020     2.715373      27.37
 C       5.635107    -1.073533     1.836409      90.30
 O       6.199965     0.112647     2.122660     312.07
 H       6.046335     0.275035     3.017279      32.30
 H       5.845991    -1.211913     0.839968      32.10
 H       6.065072    -2.098989     2.356029      28.87
55
name= lig-ACN-Water-frame_1033
 C      -3.656962    -1.278534    -2.869638      47.22
 H      -3.580807    -2.299246    -2.879120      29.16
 C      -4.601265     0.940381    -1.906087      80.64
 H      -4.881337     1.775638    -1.242068      30.00
 C      -4.369904     1.477379    -3.162079     -36.03
 O      -4.243199     2.867207    -3.485473     106.58
 C      -4.353680     3.846965    -2.294029     130.45
 H      -3.835814     4.575338    -2.781105      28.07
 H      -3.572778     3.679507    -1.607931      29.79
 H      -5.217621     3.894526    -1.770313      27.34
 C      -3.981790     0.657020    -4.326971      39.09
 O      -3.837629     1.278238    -5.509798     156.79
 H      -3.778090     2.305207    -5.429880      23.80
 C      -3.497847    -0.590178    -4.183043      45.91
 H      -2.970563    -1.174507    -5.086895      20.47
 C      -4.186940    -0.544084    -1.728019     -30.23
 C      -4.552995    -1.426291    -0.422877      76.74
 H      -5.169690    -2.189696    -0.835306      26.30
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 O      -5.242795    -0.700587     0.612949     269.47
 H      -4.584009    -0.383734     1.249660      28.17
 C      -3.105175    -2.195549     0.044934      78.36
 H      -2.710230    -2.526364    -0.977655      31.17
 C      -3.349656    -3.352929     0.985060     110.32
 O      -3.751260    -4.567179     0.182979     142.62
 H      -2.885474    -4.878466    -0.207706      29.38
 H      -3.896268    -3.452407     2.014269      24.01
 H      -2.337185    -3.479386     1.518825      25.47
 C       1.243765    -1.881933     0.303094      36.15
 H       1.645371    -2.709505    -0.125518      25.67
 C       1.019341     0.456425     0.941410      56.37
 H       1.830327     1.220864     1.162724      19.33
 C      -0.450799     0.289567     1.066160      24.79
 O      -1.344850     1.193098     1.497279     193.62
 C      -0.900630     2.544702     1.733942     133.30
 H       0.079935     2.966092     2.119739      25.98
 H      -0.825188     3.202628     0.830707      28.31
 H      -1.732062     3.097658     2.276506      28.90
 C      -0.905592    -1.075341     0.670570     -13.29
 O      -2.396599    -1.224211     0.788892     131.03
 C      -0.200624    -2.160433     0.262204      65.74
 H      -0.901911    -3.038274    -0.123936      25.76
 C       1.824037    -0.649875     0.630570      22.52
 C       3.351527    -0.679310     0.561238      79.55
 H       3.899540    -1.162712    -0.389707      23.53
 O       3.720305     0.860651     0.560845     159.82
 H       4.061285     1.094109     1.539412      19.17
 C       3.954372    -1.197059     1.890253      69.61
 H       3.452445    -0.581886     2.690019      22.86
 O       3.735722    -2.649942     1.892197     191.51
 H       4.691654    -2.900731     2.397421      23.53
 C       5.608373    -1.172301     1.737087      60.00
 O       6.155191     0.176358     2.195230     259.43
 H       5.870078     0.410179     3.145497      28.96
 H       5.971972    -1.349641     0.817714      29.16
 H       6.088891    -1.970730     2.561374      26.92
55
name= lig-ACN-Water-frame_1034
 C      -3.679425    -1.215902    -2.861572      21.42
 H      -3.458846    -2.220463    -2.865926      22.14
 C      -4.541855     0.792353    -1.901777      30.42
 H      -4.906094     1.119120    -1.005236      17.66
 C      -4.299859     1.456810    -3.209350      16.38
 O      -4.303398     2.815720    -3.469853     157.42
 C      -4.386196     3.822574    -2.362933     127.82
 H      -4.536618     4.799222    -2.695005      29.76
 H      -3.613738     3.487657    -1.734291      29.82
 H      -5.296682     3.778091    -1.937615      29.76
 C      -3.865864     0.695258    -4.272183      23.03
 O      -3.710486     1.328758    -5.515938     132.24
 H      -3.946032     2.254290    -5.317146      17.72
 C      -3.546092    -0.650507    -4.092888      55.08
 H      -3.116785    -1.290111    -4.979896      29.04
 C      -4.332858    -0.599466    -1.780018      15.09
 C      -4.536539    -1.452502    -0.463980     105.63
 H      -5.241002    -2.238530    -0.560780      31.71
 O      -5.139435    -0.695498     0.636776     243.19
 H      -4.547970    -0.517948     1.479837      25.94
 C      -3.278303    -2.120805    -0.023484      61.28
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 H      -2.578095    -2.555605    -0.793675      29.28
 C      -3.416202    -3.424101     1.070088      91.31
 O      -3.748011    -4.610888     0.207493      70.44
 H      -2.909288    -5.261768     0.034774      27.66
 H      -4.333289    -3.110992     1.590706      27.01
 H      -2.381888    -3.521499     1.550338      26.55
 C       1.188437    -2.028067     0.289171      69.43
 H       1.937443    -2.672412     0.160969      26.59
 C       1.003116     0.458403     1.029466      50.26
 H       1.216367     1.547037     1.438635      19.90
 C      -0.384866     0.256418     0.950014      -1.63
 O      -1.261961     1.217684     1.645115     179.61
 C      -0.743872     2.569354     1.624062     124.70
 H       0.008992     2.379059     2.445605      24.14
 H      -0.699065     2.996394     0.589875      28.17
 H      -1.673233     2.941708     2.187661      27.54
 C      -1.116196    -0.945045     0.671113      14.64
 O      -2.421499    -1.151913     0.856193     131.21
 C      -0.199363    -2.078032     0.276159      39.61
 H      -0.502976    -3.106544    -0.207329      24.66
 C       1.788055    -0.724585     0.619725      -1.11
 C       3.393390    -0.589083     0.577260      85.78
 H       3.644938    -1.087534    -0.440681      25.71
 O       3.868752     0.842454     0.605775     216.08
 H       4.544828     0.984238     1.266401      21.95
 C       4.070082    -1.218120     1.762746     100.68
 H       3.679552    -0.684134     2.702074      23.12
 O       3.664711    -2.561593     1.897747     258.28
 H       4.330161    -3.250968     2.372265      26.60
 C       5.526702    -1.049996     1.823948      92.78
 O       6.127340     0.178271     2.205243     274.52
 H       5.858221     0.273782     3.271003      26.48
 H       5.840628    -1.318810     0.907462      31.53
 H       5.914774    -1.951512     2.586579      26.81
55
name= lig-ACN-Water-frame_1035
 C      -3.769044    -1.368054    -2.853870      81.85
 H      -3.302750    -2.276224    -2.525209      23.42
 C      -4.541693     0.752987    -1.878678      91.93
 H      -4.861548     1.310680    -1.110406      26.06
 C      -4.208484     1.421851    -3.052985     -37.52
 O      -4.359932     2.816055    -3.442418     179.44
 C      -4.494412     3.716542    -2.396513     133.09
 H      -4.369444     4.632135    -2.927016      26.58
 H      -3.688822     3.913932    -1.684730      28.61
 H      -5.233824     3.440387    -1.764051      26.81
 C      -3.736652     0.747357    -4.279104      -4.76
 O      -3.576916     1.366476    -5.540638     109.78
 H      -3.806868     2.294656    -5.526521      19.80
 C      -3.562926    -0.691468    -4.109749      31.48
 H      -3.232294    -1.255360    -5.021710      25.28
 C      -4.395126    -0.719665    -1.781644      16.18
 C      -4.561580    -1.419897    -0.461260      98.17
 H      -5.226591    -2.170757    -0.798867      28.42
 O      -5.071433    -0.681732     0.645003     282.28
 H      -4.229308    -0.374545     1.088477      27.22
 C      -3.229239    -2.171406     0.139247      82.60
 H      -2.642891    -2.313319    -0.783596      28.94
 C      -3.544962    -3.406212     0.915911     123.14
 O      -3.745040    -4.643099     0.286296     191.66
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 H      -2.873146    -4.901839    -0.041251      29.49
 H      -4.414425    -3.326685     1.561056      26.26
 H      -2.916894    -3.579796     1.843738      25.81
 C       1.213746    -1.923832     0.303426      45.75
 H       1.514838    -2.889927     0.133768      25.53
 C       0.946785     0.243201     1.009965      60.15
 H       1.649707     1.247224     1.230235      20.39
 C      -0.472910     0.227991     1.029986      16.62
 O      -1.180627     1.157571     1.671032     186.66
 C      -0.680309     2.584479     1.676446     122.68
 H       0.290844     3.004584     2.152523      25.46
 H      -0.249768     2.723701     0.678638      28.69
 H      -1.253069     3.545818     1.820599      27.32
 C      -1.083398    -0.987939     0.570294      -9.14
 O      -2.545240    -1.034848     0.879749     122.61
 C      -0.237787    -2.005581     0.258793      55.53
 H      -0.778852    -2.987442     0.185501      26.87
 C       1.851211    -0.676536     0.642238      29.72
 C       3.335058    -0.417494     0.604845     103.12
 H       3.797582    -1.006227    -0.288091      22.54
 O       3.963220     0.801272     0.537885     259.60
 H       4.530598     0.918402     1.302656      19.06
 C       4.056254    -1.200983     1.817787      60.62
 H       3.700676    -0.623231     2.747069      20.52
 O       3.560811    -2.602233     1.866453     298.26
 H       3.981750    -2.931784     2.600848      30.67
 C       5.645505    -1.091064     1.846357      86.47
 O       6.108161     0.214856     2.236405     345.56
 H       6.086975     0.443477     3.289315      28.82
 H       6.177482    -1.175048     0.978561      30.10
 H       6.022911    -1.958704     2.641091      24.90
55
name= lig-ACN-Water-frame_1036
 C      -3.843764    -1.467938    -2.935157      50.43
 H      -3.710146    -2.567040    -3.185014      23.79
 C      -4.576250     0.771483    -1.861062      67.80
 H      -4.900893     1.383665    -1.042881      32.13
 C      -4.090699     1.418188    -3.121987     -10.88
 O      -4.339746     2.689575    -3.379109     143.00
 C      -4.589891     3.764725    -2.299041     108.13
 H      -4.990786     4.648473    -2.803861      24.81
 H      -3.566015     3.703619    -1.964479      25.23
 H      -5.422294     3.695609    -1.699190      23.14
 C      -3.674818     0.664972    -4.232477      38.82
 O      -3.454477     1.308750    -5.489061     154.29
 H      -3.433144     2.327917    -5.287241      22.19
 C      -3.542755    -0.700458    -4.146215      59.69
 H      -3.120857    -1.229659    -4.957350      25.28
 C      -4.314492    -0.689605    -1.755534     -27.32
 C      -4.591074    -1.499012    -0.410230      84.15
 H      -5.326269    -2.274905    -0.342898      25.21
 O      -5.045758    -0.635942     0.650578     240.35
 H      -4.491559     0.107139     0.775419      31.17
 C      -3.189717    -2.103660     0.118628      74.08
 H      -2.488526    -2.567690    -0.565980      28.60
 C      -3.720219    -3.348850     1.048438      91.67
 O      -3.673640    -4.685553     0.268843     151.33
 H      -3.184497    -4.706914    -0.514449      32.28
 H      -4.693398    -3.137849     1.275541      26.65
 H      -2.926354    -3.366308     1.816800      25.65
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 C       1.157124    -1.910542     0.258869      69.60
 H       1.904800    -2.655074    -0.031620      25.16
 C       0.941712     0.289992     0.998262      37.83
 H       1.306893     1.413564     1.445134      20.63
 C      -0.459384     0.169665     1.143494      21.28
 O      -1.191306     1.268903     1.762114     159.15
 C      -0.498754     2.583460     1.572740     118.65
 H      -0.068161     2.596181     2.594105      25.64
 H      -0.062734     2.760262     0.574230      27.92
 H      -1.578720     2.856632     1.633500      25.89
 C      -1.160300    -0.891533     0.632453      -5.32
 O      -2.559689    -1.031886     0.833858     133.44
 C      -0.243081    -2.052522     0.254279      39.95
 H      -0.565440    -3.050563     0.096370      26.39
 C       1.844195    -0.748255     0.593928       8.51
 C       3.466763    -0.586859     0.644573      78.20
 H       3.681728    -1.100656    -0.318056      23.56
 O       4.006619     0.896833     0.449000     202.79
 H       4.052934     1.357148     1.389953      18.58
 C       4.008476    -1.198678     1.896040      82.21
 H       3.629099    -0.695208     2.858039      19.93
 O       3.500113    -2.598801     1.860889     271.81
 H       3.743964    -3.086459     2.703019      28.31
 C       5.757601    -1.187825     1.852502      68.95
 O       6.140388     0.281191     2.266326     327.53
 H       5.966602     0.246072     3.246182      27.93
 H       6.019409    -1.543434     0.846940      28.71
 H       6.234699    -1.909767     2.669719      27.10
55
name= lig-ACN-Water-frame_1037
 C      -3.958825    -1.380006    -2.998624      62.69
 H      -4.352855    -2.462386    -2.846654      29.51
 C      -4.438876     0.637552    -1.947421      90.36
 H      -4.974697     1.151878    -1.070677      28.06
 C      -4.129886     1.310859    -3.061743       4.67
 O      -4.380120     2.741702    -3.327281     161.54
 C      -4.617630     3.759410    -2.274152     106.88
 H      -4.898471     4.646603    -2.884268      24.31
 H      -3.825635     4.250465    -1.601832      26.51
 H      -5.099237     3.141826    -1.484220      24.10
 C      -3.602012     0.624286    -4.216203       3.67
 O      -3.346223     1.215487    -5.379743     139.26
 H      -2.997708     2.150195    -5.276689      22.36
 C      -3.489817    -0.826103    -4.156007      67.24
 H      -3.232858    -1.294672    -5.010025      22.19
 C      -4.275297    -0.730329    -1.820293      21.85
 C      -4.523392    -1.447894    -0.422529      86.85
 H      -5.260452    -2.218860    -0.700946      29.44
 O      -5.103378    -0.572457     0.651836     180.55
 H      -4.501261     0.258807     0.596129      28.49
 C      -3.295973    -2.166176     0.113017      82.85
 H      -2.741218    -2.498739    -0.748917      31.44
 C      -3.733017    -3.306991     1.108915     110.53
 O      -3.599093    -4.626091     0.299180      53.70
 H      -3.394861    -4.269714    -0.671347      31.46
 H      -4.704627    -3.195473     1.382335      29.55
 H      -3.361178    -3.593051     2.075248      26.57
 C       1.152623    -1.946454     0.153513      25.26
 H       1.660452    -2.932286    -0.241674      23.09
 C       1.001966     0.398821     1.067959      56.12
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 H       1.534702     1.437252     1.508957      19.75
 C      -0.425085     0.222996     1.248265      15.04
 O      -1.149725     1.260099     1.749994     193.91
 C      -0.563991     2.591496     1.583496     123.15
 H       0.147208     2.977539     2.395729      27.32
 H       0.241558     2.605333     0.833004      28.43
 H      -0.997639     3.629096     1.466868      27.15
 C      -1.117479    -1.020937     0.755649      12.01
 O      -2.502732    -1.048940     0.773162      95.16
 C      -0.281709    -2.069867     0.265969      74.93
 H      -0.717112    -2.858032    -0.231186      30.75
 C       1.786615    -0.665805     0.595396     -12.15
 C       3.521926    -0.568512     0.604456      75.29
 H       4.122786    -1.143456    -0.074895      24.92
 O       3.933028     0.846382     0.394592     222.88
 H       3.725187     1.290506     1.332865      21.16
 C       4.171361    -1.310315     1.973301      69.96
 H       3.814168    -0.684993     2.878143      23.63
 O       3.475675    -2.571176     1.890613     253.02
 H       3.854042    -3.354012     2.620693      25.37
 C       5.656009    -1.096695     1.968046      94.53
 O       6.192952     0.146018     2.185984     354.19
 H       6.116876     0.342479     3.095624      33.95
 H       6.076069    -1.176804     0.895804      29.13
 H       6.111737    -1.958240     2.613184      26.40
55
name= lig-ACN-Water-frame_1038
 C      -4.083156    -1.550145    -2.992459      50.59
 H      -3.976694    -2.726857    -3.099802      28.98
 C      -4.341489     0.619783    -1.867136      58.59
 H      -4.759340     1.271767    -0.936474      24.30
 C      -4.154639     1.382817    -3.123241      29.79
 O      -4.342819     2.757554    -3.311453     149.43
 C      -4.626918     3.672859    -2.199300     115.90
 H      -5.473725     4.332441    -2.568359      25.95
 H      -3.570971     4.094308    -1.980920      27.11
 H      -5.422730     3.410241    -1.417520      23.11
 C      -3.541363     0.560232    -4.142935       5.26
 O      -3.202678     1.149565    -5.377325     185.16
 H      -3.084747     2.084743    -5.340006      23.59
 C      -3.521126    -0.848305    -4.170656      23.71
 H      -3.342881    -1.419337    -4.998581      19.69
 C      -4.271527    -0.748300    -1.785677      29.00
 C      -4.581052    -1.339640    -0.478150      79.46
 H      -5.365761    -2.140593    -0.582379      25.69
 O      -5.159507    -0.542255     0.538623     219.86
 H      -4.504776     0.103795     0.950486      28.02
 C      -3.294249    -2.160291     0.210040      63.21
 H      -2.837712    -2.679508    -0.621200      32.34
 C      -3.756286    -3.367872     1.087944     137.79
 O      -3.550141    -4.510944     0.372554     111.80
 H      -3.310065    -4.372940    -0.617832      31.09
 H      -4.732235    -3.244749     1.341991      30.24
 H      -3.067243    -3.199785     1.877853      27.93
 C       1.132304    -1.836812     0.112989      57.60
 H       1.789858    -2.725193    -0.419030      24.59
 C       1.066984     0.317338     1.146268      52.07
 H       1.758343     1.227324     1.442385      19.81
 C      -0.345425     0.216439     1.262791     -11.86
 O      -1.203953     1.324210     1.724881     153.08
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 C      -0.481544     2.670528     1.614041     100.95
 H      -0.039095     2.783513     2.619568      25.69
 H       0.125780     2.522088     0.700736      26.46
 H      -1.465917     3.221247     1.298414      26.43
 C      -0.949835    -1.038129     0.918096     -34.46
 O      -2.481750    -1.078200     0.733741      53.70
 C      -0.259634    -2.066178     0.199583      70.00
 H      -0.823385    -2.840367    -0.182287      28.60
 C       1.885487    -0.735491     0.549983      15.37
 C       3.438458    -0.554766     0.642530      96.82
 H       3.624100    -1.078280    -0.245170      25.98
 O       3.811284     0.745847     0.404892     253.69
 H       3.998562     1.262373     1.200900      26.81
 C       4.071641    -1.197099     1.985914      91.64
 H       3.722036    -0.754543     2.979906      24.05
 O       3.540295    -2.592489     1.942314     284.96
 H       4.252011    -3.126944     2.495398      28.12
 C       5.678751    -1.224333     1.924258      79.95
 O       6.268183     0.116146     2.166453     321.46
 H       6.031499     0.336440     3.110277      32.77
 H       5.944767    -1.798474     0.903192      27.95
 H       6.108098    -1.922311     2.733476      28.12
55
name= lig-ACN-Water-frame_1039
 C      -4.036613    -1.635081    -2.991315      61.73
 H      -3.941431    -2.804084    -2.959631      22.38
 C      -4.298276     0.752180    -1.872173      72.86
 H      -4.337144     1.272678    -0.781630      23.13
 C      -4.072285     1.340060    -3.082663      14.89
 O      -4.301538     2.685667    -3.330086     163.17
 C      -4.708350     3.609388    -2.157083      98.83
 H      -5.223567     4.493590    -2.623715      23.70
 H      -3.712220     4.212298    -1.832859      26.50
 H      -4.662417     2.919903    -1.224188      21.56
 C      -3.564721     0.571613    -4.174797      -4.48
 O      -3.067768     1.065077    -5.404833     106.09
 H      -3.364465     2.033010    -5.409572      17.89
 C      -3.687174    -0.870270    -4.063089      20.72
 H      -3.198806    -1.242463    -4.935181      30.54
 C      -4.307989    -0.755732    -1.841069     -37.50
 C      -4.592736    -1.454248    -0.400431      78.28
 H      -5.312672    -2.343123    -0.569250      27.55
 O      -5.241339    -0.448442     0.455087     221.68
 H      -4.584542    -0.288706     1.098510      29.85
 C      -3.303462    -2.060802     0.150175      88.92
 H      -2.637186    -2.445294    -0.600501      32.58
 C      -3.710247    -3.203790     1.146797     107.56
 O      -3.517124    -4.581086     0.405108     137.45
 H      -2.928795    -4.462663    -0.277471      34.96
 H      -4.664124    -3.271032     1.538339      28.99
 H      -3.077846    -3.406286     1.973637      26.85
 C       1.207038    -1.870055    -0.002614      52.87
 H       1.939979    -2.628040    -0.650324      24.79
 C       1.114361     0.246582     1.229920      56.78
 H       1.470930     1.208216     1.627408      22.44
 C      -0.335374     0.200845     1.312858     -12.46
 O      -1.157464     1.284821     1.655799     179.50
 C      -0.536432     2.632630     1.602138     122.35
 H      -0.013786     2.934000     2.534914      27.87
 H       0.172559     3.121656     0.881642      27.59
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 H      -1.332768     3.450582     1.668733      28.08
 C      -1.043371    -1.017556     0.895542      13.98
 O      -2.393418    -1.045990     0.804527     110.26
 C      -0.158124    -1.969368     0.212613      49.18
 H      -0.429583    -2.962520    -0.100851      25.98
 C       1.849450    -0.756509     0.651161      30.24
 C       3.291083    -0.701311     0.652084     108.01
 H       3.850775    -1.340521     0.036908      25.90
 O       3.734716     0.781292     0.425076     188.82
 H       4.059861     0.995252     1.271779      26.66
 C       3.953198    -1.182386     1.903752      84.78
 H       3.621673    -0.477620     2.738100      24.30
 O       3.663621    -2.594702     2.021158     300.17
 H       4.218193    -3.077565     2.523406      31.35
 C       5.662059    -1.321861     1.917221      60.99
 O       6.316801     0.064327     2.122227     308.54
 H       6.137891     0.051065     3.190353      28.77
 H       6.070792    -1.686705     0.783831      26.61
 H       5.855946    -1.974300     2.761737      28.21
55
name= lig-ACN-Water-frame_1040
 C      -4.007216    -1.489918    -2.844550      10.25
 H      -4.226665    -2.596190    -2.757164      19.15
 C      -4.237767     0.561521    -1.875397      53.64
 H      -4.434165     1.219608    -0.947566      23.19
 C      -3.971459     1.340432    -3.067027     -12.77
 O      -4.260508     2.694380    -3.330064     170.28
 C      -4.571331     3.517104    -2.175484     113.42
 H      -5.650526     3.821054    -2.322616      22.85
 H      -3.755219     4.330711    -1.909801      25.52
 H      -5.213009     2.955077    -1.308065      19.29
 C      -3.664031     0.515425    -4.231952       3.66
 O      -3.025194     0.962971    -5.366482     152.99
 H      -3.220840     1.916204    -5.693922      25.33
 C      -3.687263    -0.862824    -4.162097      67.20
 H      -3.400622    -1.567447    -4.995379      28.27
 C      -4.386723    -0.771024    -1.752188      87.06
 C      -4.567666    -1.417854    -0.478040      78.10
 H      -5.151763    -2.422486    -0.631436      27.89
 O      -5.290191    -0.412365     0.413335     143.86
 H      -4.923828    -0.341256     1.359785      25.70
 C      -3.209959    -2.023368     0.184206      68.12
 H      -2.808669    -2.409926    -0.750700      31.34
 C      -3.530597    -3.204944     1.178649     101.39
 O      -3.522174    -4.578097     0.474676     124.66
 H      -2.599667    -4.744446     0.076362      28.86
 H      -4.572214    -2.994571     1.394350      27.03
 H      -2.953550    -3.027770     2.065631      27.09
 C       1.263436    -1.825473    -0.002812      64.85
 H       1.672034    -2.792679    -0.595909      25.09
 C       1.006300     0.258572     1.390012      73.76
 H       1.704974     1.002979     1.737947      19.70
 C      -0.381333     0.140631     1.307544      27.75
 O      -1.088141     1.276204     1.550969     160.62
 C      -0.590704     2.678334     1.705852     110.71
 H       0.117030     2.600761     2.514648      26.74
 H      -0.077174     2.483275     0.745992      27.62
 H      -1.481391     3.358865     1.690738      27.54
 C      -0.960004    -1.010949     0.704851       0.13
 O      -2.446845    -0.952590     0.936156      83.85
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 C      -0.156080    -2.005508     0.218144      73.07
 H      -0.842416    -2.794321    -0.185892      29.63
 C       1.803356    -0.816061     0.676161       0.26
 C       3.406991    -0.696678     0.571256      83.52
 H       3.569130    -1.094793    -0.374862      27.22
 O       3.661883     0.718444     0.461951     198.96
 H       3.971076     1.221235     1.331053      24.46
 C       4.103922    -1.284442     1.927582      95.47
 H       3.701866    -0.726540     2.824852      25.20
 O       3.675121    -2.623242     2.100481     254.87
 H       4.198691    -2.965305     2.894277      28.93
 C       5.524198    -1.153484     1.904565      85.41
 O       6.320278    -0.096134     2.109923     313.01
 H       6.512035     0.219274     3.058267      31.34
 H       5.958870    -1.649040     0.782734      25.62
 H       5.903025    -1.957540     2.536782      26.46
55
name= lig-ACN-Water-frame_1041
 C      -4.058247    -1.490264    -2.921193      86.30
 H      -4.054999    -2.571705    -2.983452      29.27
 C      -4.231552     0.693831    -1.853277      58.76
 H      -4.622546     1.203293    -1.009912      26.02
 C      -3.965911     1.237446    -3.125239      26.06
 O      -4.134195     2.641750    -3.284380     193.48
 C      -4.644286     3.432746    -2.186361     108.71
 H      -5.351566     4.157752    -2.630785      25.12
 H      -3.773751     4.282045    -2.014236      25.63
 H      -4.434616     2.842907    -1.180292      24.42
 C      -3.668397     0.457028    -4.259331      21.55
 O      -3.028891     0.902724    -5.407682     173.65
 H      -3.068372     1.860393    -5.404768      30.11
 C      -3.696775    -0.963904    -4.102217       3.76
 H      -3.615555    -1.602797    -5.093867      12.58
 C      -4.313846    -0.736014    -1.753849      -2.29
 C      -4.545079    -1.369678    -0.314595      73.14
 H      -5.299068    -2.271909    -0.445612      26.80
 O      -5.339391    -0.457804     0.377625     184.56
 H      -5.073355    -0.602688     1.344646      27.86
 C      -3.150033    -1.959084     0.234934     102.27
 H      -2.389270    -2.243590    -0.502481      27.05
 C      -3.393721    -3.204778     1.136741     101.92
 O      -3.495929    -4.466482     0.608810     122.57
 H      -2.599211    -4.933423     0.265775      26.51
 H      -4.374855    -3.248093     1.665270      26.54
 H      -2.654457    -3.312949     1.964851      25.21
 C       1.106672    -1.904890     0.082636      30.59
 H       1.977519    -2.507775    -0.364343      26.02
 C       1.112138     0.096481     1.429255      70.73
 H       1.329585     0.990418     2.011765      21.76
 C      -0.302904     0.215689     1.245838       0.33
 O      -1.253475     1.250621     1.544030     160.31
 C      -0.525887     2.559639     1.695347     130.60
 H       0.009402     2.849199     2.593216      28.78
 H      -0.101609     3.285375     0.920414      28.92
 H      -1.382435     3.137336     1.959211      29.43
 C      -1.025951    -0.892768     0.684601     -35.85
 O      -2.441496    -0.958199     0.940710     112.39
 C      -0.291385    -2.099511     0.109031      51.52
 H      -0.572524    -3.050869    -0.514694      25.08
 C       1.884655    -0.790654     0.737752      17.22
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 C       3.366252    -0.640452     0.645658      97.64
 H       3.817490    -1.135618    -0.154189      28.64
 O       3.682716     0.734536     0.472067     191.90
 H       3.531913     1.158231     1.444842      23.56
 C       4.025254    -1.261679     1.922044      86.17
 H       3.648491    -0.546993     2.699157      26.28
 O       3.654480    -2.693661     2.158792     224.19
 H       4.127614    -3.334636     2.958338      25.65
 C       5.655693    -1.320087     1.830582      63.94
 O       6.389631    -0.027396     2.113704     300.74
 H       6.144081    -0.023768     3.033514      32.09
 H       5.779978    -1.551504     0.575426      26.21
 H       5.964422    -2.096213     2.478922      29.27
55
name= lig-ACN-Water-frame_1042
 C      -4.138652    -1.660314    -2.874133      47.52
 H      -4.119241    -2.672850    -2.630437      26.23
 C      -4.292540     0.695673    -1.876425     102.20
 H      -4.429204     1.282857    -1.112322      29.97
 C      -4.048032     1.225377    -3.117392      15.96
 O      -3.972885     2.559333    -3.309830     161.62
 C      -4.546440     3.492381    -2.227340      96.40
 H      -5.611291     3.701898    -2.349907      24.04
 H      -3.707007     4.334337    -2.196713      24.81
 H      -4.879847     3.047181    -1.158076      23.43
 C      -3.549110     0.396474    -4.252736      -7.62
 O      -3.097329     0.913656    -5.471231     156.28
 H      -2.923055     1.870018    -5.392884      20.76
 C      -3.756220    -0.996942    -4.146305      13.12
 H      -3.323607    -1.645221    -5.087460      25.26
 C      -4.192469    -0.721492    -1.756242       0.43
 C      -4.491039    -1.426702    -0.352198      82.82
 H      -4.933789    -2.499037    -0.599457      26.09
 O      -5.368857    -0.472621     0.474143     128.57
 H      -5.260634    -0.476148     1.396569      28.81
 C      -3.169432    -1.936784     0.260314      74.79
 H      -2.901122    -2.294637    -0.764972      32.84
 C      -3.266928    -3.134627     1.303035     114.01
 O      -3.485530    -4.495232     0.626607     130.65
 H      -2.720663    -4.526143     0.075576      32.87
 H      -4.033009    -2.763131     2.105482      26.16
 H      -2.267345    -3.038786     1.788108      27.35
 C       1.111784    -1.945283     0.194969      69.64
 H       1.414847    -2.813304    -0.371832      25.29
 C       1.039756     0.164648     1.472584      57.54
 H       1.831985     0.740057     2.023842      19.16
 C      -0.358004     0.151687     1.137786      -2.40
 O      -1.222039     1.258427     1.555782     145.22
 C      -0.625252     2.582282     1.800497     113.41
 H       0.187956     2.221265     2.421186      27.37
 H      -0.059013     2.637891     0.745800      27.77
 H      -1.309044     3.263988     2.090927      29.39
 C      -1.068988    -1.028314     0.666296      38.28
 O      -2.380046    -0.896871     0.933510     135.18
 C      -0.327650    -1.952578     0.076933      78.41
 H      -0.915715    -2.898867    -0.299757      30.04
 C       1.769983    -0.916238     0.743006      28.15
 C       3.350234    -0.723670     0.754686      75.98
 H       3.689568    -1.210547    -0.078295      27.57
 O       3.749748     0.804751     0.516134     161.26
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 H       3.556393     1.435775     1.225110      26.16
 C       4.071848    -1.300297     2.022078      71.27
 H       3.953697    -0.774445     2.999906      24.66
 O       3.548428    -2.675486     2.134530     251.58
 H       4.392755    -3.054923     2.620923      26.98
 C       5.740274    -1.394441     1.735630      67.62
 O       6.397996    -0.033048     2.128804     233.21
 H       6.253226     0.245590     3.010349      33.16
 H       6.369300    -1.611713     0.638409      26.66
 H       6.148309    -2.124445     2.323971      30.83
55
name= lig-ACN-Water-frame_1043
 C      -4.098176    -1.606135    -2.845331      51.32
 H      -4.291045    -2.610105    -2.877867      22.56
 C      -4.307383     0.506733    -1.897276      72.07
 H      -4.370983     1.035011    -1.048560      29.03
 C      -4.009433     1.191094    -3.193027      14.90
 O      -3.859011     2.622284    -3.304765     174.17
 C      -4.479540     3.509102    -2.339433     107.34
 H      -5.334185     3.756592    -2.895211      26.76
 H      -4.072910     4.641220    -2.319007      24.46
 H      -4.357570     3.020782    -1.308126      24.58
 C      -3.552712     0.367694    -4.214506     -25.77
 O      -3.204908     0.925429    -5.483064     127.36
 H      -3.039632     1.952746    -5.462218      17.09
 C      -3.764895    -1.121907    -4.097422      24.52
 H      -3.369561    -1.844084    -4.987379      27.60
 C      -4.264589    -0.838484    -1.699435      77.65
 C      -4.489592    -1.393941    -0.370245      92.57
 H      -5.313701    -2.208635    -0.535039      27.88
 O      -5.373012    -0.556706     0.514388     190.49
 H      -4.814630    -0.669181     1.350323      28.52
 C      -3.233725    -1.982247     0.308879     118.73
 H      -2.458021    -2.416868    -0.328019      30.15
 C      -3.135448    -3.054821     1.396054      94.18
 O      -3.459719    -4.412806     0.680450     157.92
 H      -3.196186    -4.396428    -0.223154      34.73
 H      -3.882480    -3.194575     2.328565      25.13
 H      -2.052706    -3.204348     1.750028      26.43
 C       1.079920    -2.080464     0.148003      56.68
 H       1.725840    -2.807794    -0.108063      28.26
 C       0.949457     0.113842     1.317220      72.89
 H       1.232049     1.133471     1.829434      22.34
 C      -0.407982     0.237280     1.247781      50.88
 O      -1.236719     1.199601     1.576157     216.11
 C      -0.556990     2.455856     1.846874     128.85
 H       0.101532     2.738023     2.704450      27.52
 H      -0.185094     3.059976     0.815141      27.69
 H      -1.334499     3.080390     2.085587      30.31
 C      -1.026872    -0.845686     0.758491       2.95
 O      -2.453446    -0.874341     0.832011     117.07
 C      -0.304456    -2.001187     0.082568      52.16
 H      -0.852852    -2.904661    -0.360827      27.41
 C       1.730403    -0.919264     0.896303      14.13
 C       3.373813    -0.643051     0.869707      85.50
 H       3.640912    -1.135251     0.010794      29.19
 O       3.779567     0.719229     0.541258     225.03
 H       3.850722     1.055462     1.414036      26.84
 C       4.287425    -1.403549     1.993075      83.10
 H       4.166959    -0.822724     2.944214      25.49
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 O       3.498182    -2.609577     2.115344     353.12
 H       3.825250    -3.424618     2.314094      32.86
 C       5.792984    -1.279155     1.808033      96.43
 O       6.389579    -0.115387     2.086911     330.42
 H       6.195925    -0.097818     3.080894      29.99
 H       5.771459    -1.492085     0.557449      28.32
 H       6.155502    -2.042663     2.372571      29.78
55
name= lig-ACN-Water-frame_1044
 C      -4.055871    -1.712499    -2.885803      60.70
 H      -4.169707    -2.757857    -2.827472      27.58
 C      -4.247271     0.572492    -1.929273      75.80
 H      -4.614039     1.166500    -1.097701      26.38
 C      -3.921836     1.151508    -3.096574      -8.09
 O      -3.744304     2.577028    -3.342273     187.15
 C      -4.483805     3.555944    -2.511641     126.29
 H      -5.518526     3.622517    -2.416754      25.98
 H      -3.701503     4.387516    -2.711079      24.82
 H      -4.428392     3.278455    -1.402003      27.47
 C      -3.664182     0.313598    -4.302766      31.35
 O      -3.317190     0.887951    -5.459384     153.27
 H      -3.412999     1.842002    -5.216426      27.18
 C      -3.663367    -1.037090    -4.065211      45.45
 H      -3.727559    -1.746081    -4.962694      12.03
 C      -4.377607    -0.896013    -1.742498     -38.50
 C      -4.664401    -1.550684    -0.284034      90.17
 H      -5.128817    -2.621481    -0.458736      26.71
 O      -5.287602    -0.644260     0.578337     176.60
 H      -4.773858    -0.275313     1.371752      26.45
 C      -3.145776    -2.016548     0.366055      63.57
 H      -2.912113    -2.418183    -0.639616      32.09
 C      -3.123412    -3.188298     1.387797     112.94
 O      -3.458574    -4.314699     0.762888     153.29
 H      -3.320946    -4.147355    -0.292414      28.22
 H      -3.791755    -2.936211     2.431290      23.89
 H      -2.005316    -3.134420     1.737832      25.04
 C       1.188909    -1.989306     0.278068      56.39
 H       1.614112    -2.767181    -0.112059      26.97
 C       0.999461     0.226042     1.250180      45.16
 H       1.749564     1.143639     1.404235      18.47
 C      -0.458569     0.153620     1.314768      -0.13
 O      -1.254086     1.294705     1.697573     131.37
 C      -0.589520     2.533258     1.905445     123.92
 H      -0.050561     2.332093     2.839342      27.68
 H       0.009422     3.122259     0.949954      25.96
 H      -1.420034     3.065954     2.090107      30.38
 C      -1.163100    -0.995053     0.654262       4.76
 O      -2.528371    -0.776015     0.731889     125.04
 C      -0.305298    -2.045117     0.183751      64.06
 H      -0.750795    -2.841115    -0.403707      28.34
 C       1.840612    -0.936021     0.940306      14.14
 C       3.389763    -0.714421     0.852062      93.37
 H       3.664461    -1.281107     0.022164      25.44
 O       3.791518     0.610945     0.644598     266.87
 H       3.751498     1.277787     1.320250      25.56
 C       4.210097    -1.328016     2.050917      79.60
 H       4.061986    -0.780761     2.997760      23.82
 O       3.472587    -2.622536     2.080835     297.76
 H       4.114819    -3.241150     2.459120      29.23
 C       5.789617    -1.451830     1.726192      75.53
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 O       6.413569    -0.080009     2.104491     287.52
 H       6.340261     0.334225     3.089590      30.11
 H       6.203687    -1.507083     0.550519      26.38
 H       6.261953    -2.214939     2.141702      29.23
55
name= lig-ACN-Water-frame_1045
 C      -4.047683    -1.730513    -2.851033      53.55
 H      -3.864601    -2.812133    -2.785032      26.39
 C      -4.289141     0.522814    -1.814465      -4.22
 H      -4.588005     1.313952    -0.997901      26.02
 C      -3.830526     1.144146    -3.107660      13.13
 O      -3.733538     2.445443    -3.382379     177.18
 C      -4.406404     3.569920    -2.587893     112.66
 H      -5.329047     3.441418    -3.011841      25.52
 H      -4.292183     4.602718    -3.013701      25.28
 H      -4.051579     3.524932    -1.542497      25.03
 C      -3.739108     0.323939    -4.184270       4.00
 O      -3.440770     0.896178    -5.485903     156.32
 H      -3.554149     1.825647    -5.577208      31.16
 C      -3.666458    -1.103916    -4.134862      18.53
 H      -3.267979    -1.530975    -5.061041      15.54
 C      -4.441798    -0.923248    -1.735812      -6.15
 C      -4.622479    -1.697529    -0.238231      82.14
 H      -5.443854    -2.503151    -0.167382      26.41
 O      -5.299775    -0.704840     0.677221     220.42
 H      -4.508932    -0.255132     0.923479      33.82
 C      -3.291834    -2.021221     0.227544     103.10
 H      -2.532352    -2.385456    -0.485213      29.45
 C      -3.070094    -3.065227     1.428877      73.78
 O      -3.541190    -4.405624     0.764678     143.29
 H      -3.077058    -4.392678    -0.165623      30.31
 H      -3.976702    -2.806734     2.286067      24.59
 H      -2.043624    -3.322991     1.887536      24.22
 C       1.109965    -1.954267     0.441717      72.74
 H       1.695317    -2.630896     0.043155      28.21
 C       1.057161     0.258019     1.252223      67.60
 H       1.428325     1.363095     1.406817      20.45
 C      -0.384188     0.148994     1.276394     -23.06
 O      -1.263346     1.267123     1.743201     119.57
 C      -0.638570     2.642409     2.059142     111.42
 H       0.080667     2.702975     2.871599      28.83
 H       0.037520     2.651697     1.086870      26.31
 H      -1.176616     3.542071     2.202126      28.19
 C      -1.120752    -0.972971     0.705795     -11.85
 O      -2.551466    -0.796645     0.600518      96.33
 C      -0.244132    -2.040868     0.290182      74.15
 H      -0.543545    -2.945231    -0.128657      27.52
 C       1.876655    -0.799845     0.874182      23.20
 C       3.403992    -0.802692     0.830251      97.96
 H       3.785110    -1.320757    -0.041824      24.24
 O       3.818696     0.597784     0.654371     237.34
 H       3.587471     0.945900     1.525795      25.99
 C       4.049466    -1.373695     2.036318      78.19
 H       4.045919    -0.760179     2.948697      24.41
 O       3.547653    -2.678768     2.114403     246.41
 H       4.127667    -3.349719     2.806285      25.38
 C       5.816025    -1.405112     1.739162      66.02
 O       6.435001    -0.113568     2.060787     333.23
 H       6.146850    -0.145958     3.052479      29.14
 H       5.919679    -1.633637     0.555486      27.80
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 H       6.086384    -2.122958     2.349475      31.22
55
name= lig-ACN-Water-frame_1046
 C      -4.009852    -1.659207    -2.872595      44.12
 H      -3.880981    -2.786670    -2.722953      23.79
 C      -4.343936     0.429846    -1.794254      69.40
 H      -4.436540     0.939443    -0.688451      26.44
 C      -3.941555     1.043799    -2.938433     -23.81
 O      -3.703869     2.473563    -3.389529     203.43
 C      -4.394425     3.499517    -2.760929     123.05
 H      -5.386508     3.358043    -2.416676      24.31
 H      -3.996462     4.283690    -3.404080      24.67
 H      -4.120399     3.677613    -1.718965      25.79
 C      -3.694154     0.284247    -4.243208     -20.72
 O      -3.581501     0.845392    -5.498709      94.88
 H      -3.607944     1.851704    -5.237683      17.85
 C      -3.714835    -1.145403    -4.097729      92.98
 H      -3.159103    -1.806239    -4.658636      28.91
 C      -4.433989    -0.974355    -1.680966      43.22
 C      -4.705658    -1.586421    -0.322964      92.81
 H      -5.214490    -2.579368    -0.529369      26.32
 O      -5.247311    -0.792554     0.753141     174.20
 H      -4.755076     0.058522     0.881438      27.59
 C      -3.139692    -2.142009     0.183438      73.22
 H      -2.904194    -2.705973    -0.741072      30.42
 C      -3.232512    -3.044946     1.322118      97.83
 O      -3.599319    -4.461253     0.793635     176.15
 H      -2.909928    -4.788757     0.308093      33.95
 H      -3.994690    -2.982586     2.333870      23.73
 H      -2.166972    -2.965179     1.720309      24.84
 C       1.192522    -1.956105     0.523332      43.85
 H       1.666919    -2.889304     0.466930      23.62
 C       1.011430     0.364520     1.286198      74.92
 H       1.448663     1.276115     1.753075      19.72
 C      -0.397580     0.338457     1.255461      18.71
 O      -1.234094     1.243275     1.817587     169.82
 C      -0.549182     2.620802     2.091458     113.31
 H      -0.230028     2.575835     3.104108      27.39
 H       0.062650     3.238494     1.338510      26.41
 H      -1.606766     2.922713     2.083043      24.29
 C      -1.062611    -0.848739     0.815422      -4.46
 O      -2.473395    -0.833424     0.491078     106.23
 C      -0.297624    -2.040827     0.408522      43.81
 H      -0.774434    -2.926408     0.120643      26.72
 C       1.780777    -0.727531     0.789569      27.00
 C       3.349862    -0.709146     0.737516      79.18
 H       3.620619    -1.292887    -0.188581      25.75
 O       3.864510     0.556296     0.617412     210.93
 H       3.924453     1.275751     1.322401      27.34
 C       4.177308    -1.459340     2.017839      72.30
 H       3.674737    -0.908532     2.767205      27.73
 O       3.618779    -2.792325     2.197613     286.44
 H       4.095420    -3.593958     2.822717      27.32
 C       5.620355    -1.334374     1.845935     110.53
 O       6.432709    -0.204372     2.002317     325.88
 H       6.476593     0.178698     2.858143      34.06
 H       5.923545    -1.696946     0.742525      28.54
 H       6.069093    -2.050802     2.352593      29.95
55
name= lig-ACN-Water-frame_1047
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 C      -4.037858    -1.754273    -2.760169      13.56
 H      -4.046136    -2.920335    -2.749054      25.59
 C      -4.363999     0.446994    -1.766852      14.51
 H      -4.459898     1.289232    -0.871493      22.62
 C      -4.028226     1.004209    -3.110711     -19.91
 O      -3.715359     2.295291    -3.326337     160.32
 C      -4.407377     3.553694    -2.788692     106.70
 H      -5.447659     3.354371    -2.750337      23.99
 H      -4.525940     4.342340    -3.483137      26.07
 H      -3.720555     3.915990    -2.069079      26.94
 C      -3.729525     0.190116    -4.176804      25.67
 O      -3.705303     0.833429    -5.433452     153.02
 H      -3.596767     1.843347    -5.332367      22.14
 C      -3.660166    -1.148664    -4.039968      69.71
 H      -3.595500    -1.685840    -4.916496      18.87
 C      -4.427062    -0.922376    -1.692252      28.37
 C      -4.573463    -1.574218    -0.354712      83.52
 H      -5.318158    -2.385663    -0.339140      26.92
 O      -5.225677    -0.895955     0.768898     170.58
 H      -4.833704     0.054465     0.857156      28.10
 C      -3.182731    -2.099433     0.061057      80.30
 H      -2.563789    -2.530945    -0.741107      30.15
 C      -3.341473    -3.206587     1.261871     103.99
 O      -3.637769    -4.473656     0.854567     178.58
 H      -2.723731    -4.862938     0.618587      30.56
 H      -4.294491    -2.600956     1.821894      24.78
 H      -2.502933    -3.360158     1.988099      26.11
 C       1.095920    -1.979938     0.563325      58.44
 H       1.807113    -2.878853     0.490243      21.26
 C       1.001071     0.447641     1.275825      70.24
 H       1.602597     1.145524     1.685413      21.25
 C      -0.400741     0.344564     1.246190      14.33
 O      -1.147464     1.351723     1.883544     218.38
 C      -0.704465     2.605899     2.188475     119.57
 H      -0.163176     2.529241     3.126957      27.83
 H       0.152878     2.744693     1.487620      26.61
 H      -1.334982     3.663252     2.261189      24.36
 C      -1.056083    -0.878080     0.730783      29.70
 O      -2.363255    -0.905008     0.420220     177.05
 C      -0.230607    -1.972943     0.610222      79.02
 H      -0.770005    -2.848692     0.274474      27.35
 C       1.754115    -0.710155     0.813651      30.67
 C       3.290171    -0.727592     0.741218      76.80
 H       3.548955    -1.213959    -0.284405      22.82
 O       3.967845     0.624987     0.512913     174.92
 H       3.461375     1.041508     1.269018      26.11
 C       3.974727    -1.425468     2.035453     103.48
 H       3.983503    -0.867134     2.945925      25.49
 O       3.659922    -2.876053     2.210573     278.35
 H       4.471694    -3.292029     2.466092      28.50
 C       5.628750    -1.514380     1.890406      85.36
 O       6.446973    -0.141454     1.958723     290.06
 H       6.193862     0.103165     2.846189      32.16
 H       5.757369    -1.757058     0.779430      27.07
 H       5.914251    -2.203705     2.554627      31.94
55
name= lig-ACN-Water-frame_1048
 C      -4.072787    -1.817734    -2.765874      53.14
 H      -4.148446    -2.939611    -2.504924      29.46
 C      -4.360960     0.553986    -1.883526      93.73
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 H      -4.648790     1.310707    -1.029799      25.71
 C      -4.117018     1.008312    -3.076074      28.53
 O      -3.737551     2.317988    -3.316654     225.38
 C      -4.436267     3.552942    -2.836729     116.53
 H      -5.267089     3.236342    -2.234868      25.78
 H      -4.457128     3.973991    -3.768812      25.36
 H      -4.037701     4.064404    -2.037564      29.13
 C      -3.844174     0.170827    -4.185014       5.91
 O      -3.777484     0.781895    -5.409383     134.90
 H      -3.652069     1.696738    -5.179605      23.32
 C      -3.687111    -1.289281    -3.975806       9.32
 H      -3.504501    -1.888745    -4.880787       8.39
 C      -4.411666    -0.872528    -1.668198     -50.25
 C      -4.513585    -1.658687    -0.310597      86.43
 H      -4.955392    -2.602368    -0.597290      28.04
 O      -5.199654    -0.932183     0.744286     208.75
 H      -4.611092    -0.224908     0.969609      31.93
 C      -3.064401    -2.158040     0.058745      81.90
 H      -2.730301    -2.661206    -0.855050      33.07
 C      -3.422017    -3.116649     1.277704      86.33
 O      -3.696692    -4.596983     0.825016      99.96
 H      -2.802794    -5.103922     0.527418      29.60
 H      -4.507809    -3.017631     1.744617      24.80
 H      -2.723045    -2.932003     2.139621      26.34
 C       1.178625    -1.889098     0.649074      30.79
 H       1.748162    -2.875833     0.210080      21.81
 C       1.037947     0.373836     1.201583      76.19
 H       1.235225     1.326360     1.416556      26.11
 C      -0.381326     0.338742     1.277473       3.96
 O      -1.291670     1.362095     1.902754     108.67
 C      -0.583176     2.719147     2.317558      94.71
 H      -0.263515     2.778090     3.364760      27.86
 H       0.238835     2.932064     1.607771      27.62
 H      -1.511696     3.494153     1.964747      24.20
 C      -1.036098    -0.823354     0.717925       5.98
 O      -2.396824    -0.891313     0.411889     125.96
 C      -0.282463    -2.078633     0.679382      38.78
 H      -0.619585    -3.131008     0.444274      26.22
 C       1.821310    -0.711587     0.879074      50.72
 C       3.320676    -0.724038     0.779703      73.75
 H       3.723050    -1.551078     0.021694      23.51
 O       3.892029     0.597968     0.490219     250.13
 H       3.777656     1.347707     1.064954      29.19
 C       3.956661    -1.420307     2.038724      82.90
 H       3.434725    -0.902625     2.834846      25.46
 O       3.615863    -2.782479     2.158591     328.61
 H       4.276886    -3.402098     2.293271      31.99
 C       5.682433    -1.490101     1.823074      95.22
 O       6.356142    -0.226795     1.956348     301.58
 H       6.113196     0.145485     2.889556      28.67
 H       5.956417    -2.131502     0.980295      29.33
 H       6.032473    -1.959992     2.644901      29.11
55
name= lig-ACN-Water-frame_1049
 C      -4.130060    -1.737308    -2.714687      67.74
 H      -3.960087    -2.822300    -2.534054      27.09
 C      -4.461235     0.452753    -1.752423      36.59
 H      -4.586161     1.064063    -0.840171      31.00
 C      -4.106139     1.049115    -3.111654     -54.63
 O      -3.721150     2.432222    -3.347680     164.37
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 C      -4.526193     3.505474    -2.852800     123.04
 H      -5.484216     3.281282    -2.435028      22.60
 H      -4.924182     4.216899    -3.525900      26.62
 H      -3.767583     4.058584    -2.476891      26.72
 C      -3.950654     0.061001    -4.216375       5.68
 O      -3.793997     0.697676    -5.447274     136.45
 H      -3.781805     1.669858    -5.302683      25.03
 C      -3.827976    -1.299959    -4.021106      72.81
 H      -3.097163    -1.981371    -4.573847      21.12
 C      -4.390385    -0.940675    -1.625404      52.80
 C      -4.508555    -1.666636    -0.397346      69.71
 H      -5.159630    -2.503094    -0.435759      27.12
 O      -5.153199    -0.970259     0.690515     191.18
 H      -4.447130    -0.599751     1.252853      30.33
 C      -3.082031    -2.200463     0.184954      87.18
 H      -2.456547    -2.683998    -0.571304      31.90
 C      -3.477266    -3.151438     1.295182     100.15
 O      -3.682777    -4.624269     0.789923     145.56
 H      -2.901863    -4.787608     0.330479      35.31
 H      -4.465678    -2.725478     1.628215      25.56
 H      -2.721271    -3.201407     2.128312      26.30
 C       1.158793    -1.959375     0.690525      53.21
 H       1.870756    -2.955248     0.455294      21.93
 C       0.988242     0.477083     1.218039      68.62
 H       1.716553     1.205112     1.281781      23.04
 C      -0.488717     0.335419     1.320648       3.94
 O      -1.274348     1.335661     1.854897      84.02
 C      -0.503640     2.769397     2.312757      79.00
 H      -0.477104     2.535650     3.418496      27.53
 H       0.471900     3.054319     1.894233      25.73
 H      -1.549287     3.474136     2.231012      24.01
 C      -1.061716    -0.956190     0.806944       9.45
 O      -2.432980    -0.858011     0.467708     143.96
 C      -0.205687    -2.042070     0.654984      92.85
 H      -0.839910    -2.972058     0.421387      28.83
 C       1.856923    -0.736427     0.903919       6.43
 C       3.428454    -0.737664     0.818579      88.91
 H       3.549000    -1.201077    -0.273297      24.53
 O       3.785354     0.555175     0.454438     244.60
 H       3.782920     0.897155     1.356680      28.28
 C       4.164104    -1.388176     2.023474      96.40
 H       4.122326    -0.814087     2.982791      26.34
 O       3.452899    -2.694462     2.055931     256.04
 H       4.100304    -3.457805     2.507447      26.61
 C       5.575391    -1.459372     1.957905     118.77
 O       6.288049    -0.255525     1.923646     289.18
 H       6.202500     0.211179     2.907318      28.17
 H       5.801439    -1.765057     0.946343      29.38
 H       5.863281    -2.214735     2.583980      32.27
55
name= lig-ACN-Water-frame_1050
 C      -4.110706    -1.797814    -2.740661      82.16
 H      -3.841470    -2.831202    -2.588968      28.37
 C      -4.456848     0.470826    -1.775469      94.64
 H      -4.512014     1.060804    -0.935371      29.73
 C      -4.136333     0.973333    -3.024282       9.97
 O      -3.783150     2.337156    -3.425072     131.11
 C      -4.638114     3.600356    -2.851267     102.57
 H      -5.110235     3.084844    -2.053299      22.92
 H      -5.107788     3.911433    -3.745570      24.63
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 H      -4.153124     4.161064    -2.177355      26.34
 C      -4.023721     0.205910    -4.188149     -33.44
 O      -3.773098     0.589274    -5.531981      79.83
 H      -3.936327     1.615356    -5.510856      27.56
 C      -3.932923    -1.241011    -4.041542     -59.89
 H      -3.568661    -1.832458    -4.995119      16.49
 C      -4.438110    -0.932000    -1.686339       3.37
 C      -4.527242    -1.766125    -0.317645      91.98
 H      -5.075252    -2.604745    -0.618683      27.68
 O      -5.129021    -0.944676     0.686743     200.96
 H      -4.428525    -0.677739     1.397735      27.50
 C      -3.186282    -2.176749     0.221514      70.18
 H      -2.530448    -2.658355    -0.549804      29.53
 C      -3.484784    -3.290956     1.396993     116.90
 O      -3.631249    -4.507532     0.730640     188.74
 H      -3.137519    -4.563417    -0.103298      33.29
 H      -4.403577    -3.179407     1.955698      26.09
 H      -2.711118    -3.377380     2.231781      26.59
 C       1.173365    -2.027525     0.715816      34.87
 H       1.800217    -3.057460     0.778881      19.29
 C       1.000011     0.367874     1.216229      81.78
 H       1.151764     1.399761     1.516707      21.19
 C      -0.356754     0.315482     1.315798      10.66
 O      -1.158041     1.413388     1.756155     175.67
 C      -0.598331     2.627530     2.350388     132.31
 H      -0.203106     2.477155     3.443112      27.34
 H       0.368729     2.629751     1.728810      24.01
 H      -0.990803     3.733830     2.100482      25.06
 C      -1.084757    -0.887552     0.971012       2.92
 O      -2.449557    -0.919805     0.628474     131.46
 C      -0.236287    -2.029541     0.591623      38.14
 H      -0.515858    -3.069860     0.193367      24.35
 C       1.719502    -0.759752     0.979520      34.17
 C       3.348308    -0.747592     0.756616      64.05
 H       3.813618    -1.618438     0.063560      20.80
 O       3.758268     0.643982     0.486642     205.23
 H       3.857645     1.374017     1.201801      26.27
 C       4.063349    -1.336881     2.058637      66.82
 H       3.683036    -0.689800     2.897964      22.76
 O       3.365102    -2.623965     2.013907     253.94
 H       3.740120    -3.360691     2.744724      26.92
 C       5.678377    -1.645053     1.870697      89.58
 O       6.283152    -0.189387     1.968725     328.74
 H       6.133122     0.177534     2.995503      26.98
 H       5.878069    -2.092659     0.929847      29.94
 H       6.126164    -2.193057     2.653484      29.06
55
name= lig-ACN-Water-frame_1051
 C      -4.092486    -1.814325    -2.850450      39.84
 H      -4.110124    -2.877849    -2.751578      20.37
 C      -4.406946     0.464639    -1.805587      32.55
 H      -4.592202     1.064231    -0.998524      23.31
 C      -4.161294     1.070945    -3.105144     -24.07
 O      -3.912857     2.336485    -3.409872     178.99
 C      -4.703244     3.465143    -2.787836     118.41
 H      -5.533005     3.239117    -2.153990      23.79
 H      -5.306725     3.858805    -3.602665      25.99
 H      -4.037108     4.247874    -2.768994      26.17
 C      -4.030240     0.163744    -4.241353      10.01
 O      -3.780292     0.552855    -5.549177     154.46
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 H      -3.909340     1.493721    -5.685563      30.41
 C      -4.015809    -1.158340    -4.044893     126.88
 H      -4.127638    -1.740042    -5.014916      24.71
 C      -4.453422    -1.037478    -1.654885     -44.66
 C      -4.559225    -1.698856    -0.291512      94.44
 H      -5.062667    -2.603804    -0.243157      31.27
 O      -5.200249    -0.895235     0.732306     250.35
 H      -4.450693    -0.645772     1.266534      29.69
 C      -3.181733    -2.200444     0.378166      58.19
 H      -2.690302    -2.694942    -0.558888      27.76
 C      -3.409345    -3.290937     1.487110     107.40
 O      -3.601457    -4.527848     0.602950      83.22
 H      -3.213983    -4.226442    -0.367789      28.67
 H      -4.220183    -3.213913     2.088916      27.73
 H      -2.381593    -3.247090     1.943177      26.84
 C       1.079575    -2.001095     0.759443      45.10
 H       1.639476    -2.923999     0.386251      23.88
 C       1.035905     0.310607     1.282603      69.75
 H       1.900275     1.059665     1.387124      17.33
 C      -0.436937     0.276906     1.345570      17.55
 O      -1.172312     1.464403     1.644471     168.70
 C      -0.450840     2.489605     2.304814     121.59
 H      -0.518048     2.353303     3.503831      26.67
 H       0.549334     3.017452     1.925937      24.20
 H      -1.374340     3.174186     2.182225      25.85
 C      -1.058721    -0.964731     0.962966      18.71
 O      -2.498274    -0.957987     0.863506     139.34
 C      -0.333057    -2.047433     0.574676      74.80
 H      -1.002089    -2.830123     0.206627      22.97
 C       1.862326    -0.863485     0.963085      30.96
 C       3.288166    -0.601108     0.850690      90.96
 H       3.426924    -0.982934    -0.285435      20.59
 O       3.739694     0.700766     0.464377     230.94
 H       3.549458     1.167584     1.339149      25.36
 C       3.935552    -1.387481     2.012769      70.55
 H       3.816090    -0.805303     3.019562      24.99
 O       3.318234    -2.635543     2.073386     306.07
 H       3.656210    -3.097583     2.778574      33.28
 C       5.728841    -1.540173     1.843971      90.76
 O       6.290604    -0.304078     1.984479     315.47
 H       5.933808     0.087920     2.888733      28.10
 H       6.064524    -1.920236     0.985220      29.15
 H       5.991346    -2.229783     2.678374      28.43
55
name= lig-ACN-Water-frame_1052
 C      -4.211443    -1.825933    -2.772150       0.91
 H      -4.230395    -2.897754    -2.872531      14.92
 C      -4.378223     0.339113    -1.873782      77.14
 H      -4.582817     0.979707    -1.025988      26.20
 C      -4.207716     0.986387    -3.157123       1.15
 O      -4.042248     2.417413    -3.370870     214.49
 C      -4.823070     3.428611    -2.846067     128.99
 H      -4.950100     3.212618    -1.772879      25.60
 H      -5.636949     3.677591    -3.505264      25.30
 H      -4.086108     4.118675    -2.483105      26.31
 C      -4.004160     0.190150    -4.271209      -2.67
 O      -3.800572     0.591172    -5.589775     170.97
 H      -3.927442     1.544937    -5.578842      21.06
 C      -4.116653    -1.236087    -4.134916      11.74
 H      -3.886411    -1.895386    -4.936863      35.75
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 C      -4.345604    -1.003905    -1.672398      50.16
 C      -4.570486    -1.662402    -0.168093      89.29
 H      -5.240564    -2.389968    -0.455698      28.62
 O      -5.295160    -0.806526     0.778527     232.15
 H      -4.757064    -0.141889     1.208671      29.44
 C      -3.212236    -2.104405     0.461817      85.49
 H      -2.392943    -2.358407    -0.314287      25.55
 C      -3.253058    -3.301356     1.392600     117.52
 O      -3.579087    -4.548935     0.541603     162.33
 H      -3.114078    -4.444722    -0.358086      30.42
 H      -3.988659    -3.133816     2.037137      29.17
 H      -2.513030    -3.738266     2.087563      25.75
 C       1.029595    -2.105936     0.610870      48.08
 H       1.560248    -2.923913     0.191464      24.45
 C       1.008641     0.256189     1.369465      64.86
 H       1.248018     1.365654     1.469379      16.74
 C      -0.371898     0.241939     1.361381       7.51
 O      -1.168479     1.359394     1.482905     122.35
 C      -0.444284     2.544057     2.359176      86.06
 H      -0.113381     1.898407     3.322226      27.38
 H       0.630700     2.725343     1.783573      22.98
 H      -1.020306     3.505718     2.459573      25.80
 C      -1.182379    -0.914930     0.943998      13.58
 O      -2.540259    -0.996856     1.107243     176.95
 C      -0.355951    -2.080942     0.625547      55.89
 H      -0.634495    -3.047407     0.301264      24.38
 C       1.694940    -0.822017     0.977968      25.00
 C       3.318025    -0.641100     0.763165      62.61
 H       3.746998    -1.347752    -0.118030      22.68
 O       3.682326     0.790440     0.568029     225.59
 H       3.657551     1.468669     1.236457      28.90
 C       4.107662    -1.389925     1.920887      82.27
 H       3.962034    -0.707206     2.894511      24.76
 O       3.288173    -2.708489     2.160201     249.79
 H       3.812842    -3.281869     2.738389      31.18
 C       5.491489    -1.550698     1.841638     108.12
 O       6.380215    -0.330686     2.020231     228.08
 H       6.096023     0.147001     2.863762      31.91
 H       5.721488    -1.812335     0.930228      31.06
 H       5.886924    -2.347366     2.533085      28.80
55
name= lig-ACN-Water-frame_1053
 C      -4.340487    -1.870924    -2.824323      88.70
 H      -4.115805    -2.878332    -2.492421      28.68
 C      -4.372672     0.439277    -1.916998      45.27
 H      -4.408484     1.157451    -0.998662      27.00
 C      -4.253088     0.963550    -3.167702       9.50
 O      -4.080292     2.306719    -3.442850     162.63
 C      -4.942356     3.494996    -2.674973      91.41
 H      -5.325909     3.030907    -1.780403      24.18
 H      -5.975767     3.565581    -3.081689      25.63
 H      -4.535680     4.503483    -2.909675      24.58
 C      -4.032384     0.079714    -4.343009       9.28
 O      -3.821825     0.688190    -5.615215     103.87
 H      -3.912979     1.710306    -5.437463      19.31
 C      -4.132382    -1.314955    -4.089174      51.51
 H      -3.732975    -1.855075    -4.865630      22.49
 C      -4.273472    -1.044795    -1.594940     -94.85
 C      -4.560231    -1.548247    -0.116281      73.49
 H      -5.023093    -2.502756    -0.042896      26.28
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 O      -5.389103    -0.719210     0.790823     167.76
 H      -4.793760     0.130541     0.769880      29.27
 C      -3.127881    -2.061502     0.454860      50.86
 H      -2.712734    -2.231565    -0.610634      28.03
 C      -3.230902    -3.449933     1.305729     119.82
 O      -3.570103    -4.535290     0.498683     203.10
 H      -2.938611    -4.637192    -0.144909      33.34
 H      -4.023097    -3.447900     1.924563      28.24
 H      -2.232713    -3.315269     1.693114      26.12
 C       1.081389    -2.001762     0.446463      61.83
 H       1.580489    -2.883061     0.332810      24.33
 C       0.939563     0.259101     1.425162      51.34
 H       1.594632     1.096215     1.660382      16.45
 C      -0.544657     0.176584     1.301358      14.82
 O      -1.150668     1.452143     1.453473     139.62
 C      -0.434953     2.410298     2.316891      89.04
 H      -0.055445     2.141835     3.428430      25.08
 H       0.460667     3.012218     1.554242      22.45
 H      -1.205963     3.163591     2.466668      27.07
 C      -1.128974    -1.003573     1.006303      16.97
 O      -2.600559    -0.940043     1.340863     146.80
 C      -0.419949    -2.150316     0.671084      55.74
 H      -1.011706    -2.977849     0.534665      27.79
 C       1.754855    -0.897963     0.882679      13.48
 C       3.271167    -0.714052     0.743057      85.79
 H       3.599167    -0.987214    -0.328737      23.04
 O       3.625114     0.773298     0.633485     211.10
 H       3.490638     1.038928     1.542532      27.51
 C       3.912371    -1.317482     1.993422      81.09
 H       3.580311    -0.627685     2.949042      24.57
 O       3.352078    -2.694610     2.241083     199.42
 H       4.099112    -3.520847     2.368801      25.71
 C       5.569455    -1.668951     1.701581      66.42
 O       6.454486    -0.384113     2.054843     235.67
 H       6.084120     0.005981     2.921581      30.10
 H       5.696608    -1.987295     0.804730      29.66
 H       5.831635    -2.470731     2.519405      27.93
55
name= lig-ACN-Water-frame_1054
 C      -4.303067    -1.843560    -2.690655      17.88
 H      -4.316726    -2.919946    -2.810226      28.43
 C      -4.335975     0.424372    -1.838852      44.09
 H      -4.281604     1.327868    -1.011420      25.52
 C      -4.267624     0.924188    -3.236050     -19.79
 O      -4.188513     2.346634    -3.500383      96.15
 C      -5.104808     3.351976    -2.586099      91.98
 H      -4.828943     3.564976    -1.537761      23.76
 H      -6.064509     3.178185    -3.116943      23.61
 H      -4.409382     4.207959    -2.890331      24.92
 C      -4.142399     0.056761    -4.338238      33.43
 O      -3.854462     0.729354    -5.550120     136.11
 H      -3.929650     1.698319    -5.299909      25.12
 C      -4.054651    -1.350828    -4.087495       6.48
 H      -4.018479    -2.128440    -4.804388       5.87
 C      -4.461179    -0.934531    -1.608237      24.36
 C      -4.534270    -1.531583    -0.107685      89.09
 H      -5.261980    -2.333125    -0.312319      25.64
 O      -5.383631    -0.622046     0.705696     190.98
 H      -5.105071     0.301828     0.828079      30.88
 C      -3.253253    -1.988055     0.510617      92.62
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 H      -2.363734    -2.077025    -0.144564      28.26
 C      -3.224746    -3.373846     1.234709     116.08
 O      -3.539324    -4.607200     0.399595     163.84
 H      -2.858594    -4.709752    -0.368169      28.00
 H      -3.806640    -3.282159     2.122061      28.44
 H      -2.403757    -3.806711     1.764629      25.69
 C       0.973008    -2.036564     0.373526      55.95
 H       1.556750    -2.793547    -0.090851      25.53
 C       0.933055     0.118083     1.345685      83.87
 H       1.351773     0.944522     1.777655      23.53
 C      -0.423032     0.298246     1.291414       3.93
 O      -1.182284     1.448390     1.492578     186.37
 C      -0.486747     2.416838     2.221127     100.55
 H      -0.106239     1.803376     3.154718      25.24
 H       0.483617     3.185351     1.728886      22.76
 H      -1.280116     3.097266     2.577765      26.52
 C      -1.205325    -1.026405     1.208157      -0.11
 O      -2.533675    -1.039610     1.371182     145.71
 C      -0.362497    -2.148454     0.650760      56.35
 H      -0.650063    -3.169218     0.446161      26.24
 C       1.702331    -0.810008     0.782594      33.82
 C       3.165283    -0.651856     0.749012      96.00
 H       3.549119    -1.272040    -0.098588      24.38
 O       3.568203     0.628457     0.712455     278.21
 H       3.523920     1.393779     1.400962      24.41
 C       3.864541    -1.429272     1.957592      59.25
 H       4.005836    -0.598055     2.831124      25.66
 O       3.398745    -2.658017     2.322018     252.92
 H       4.244606    -3.215734     2.014022      26.04
 C       5.638927    -1.557684     1.736957      71.93
 O       6.468999    -0.594298     2.019668     245.53
 H       6.113945    -0.056120     2.840508      28.80
 H       5.820203    -1.708344     0.793455      28.64
 H       5.926632    -2.568674     2.328450      27.66
55
name= lig-ACN-Water-frame_1055
 C      -4.232082    -1.738169    -2.691404      70.76
 H      -4.243753    -2.729816    -2.264792      25.43
 C      -4.323367     0.481695    -1.903475      57.78
 H      -4.325979     1.194845    -0.889556      22.48
 C      -4.299900     0.965306    -3.127318       1.03
 O      -4.359865     2.337512    -3.454574     238.42
 C      -5.049575     3.199075    -2.667294     131.88
 H      -4.828100     2.850916    -1.643565      25.98
 H      -6.164598     3.062555    -2.367262      27.11
 H      -5.153927     4.284772    -3.129287      23.71
 C      -4.165359     0.086445    -4.268328       9.09
 O      -3.916509     0.692322    -5.477194     139.86
 H      -4.078723     1.604134    -5.304059      24.96
 C      -4.072368    -1.313017    -3.980724      71.87
 H      -3.922565    -1.996789    -4.880745      19.12
 C      -4.551285    -0.919263    -1.600415      20.20
 C      -4.692193    -1.416489    -0.214762      86.09
 H      -5.161916    -2.462367    -0.150999      27.34
 O      -5.379250    -0.553095     0.632910     241.40
 H      -4.699922     0.111454     0.764469      29.32
 C      -3.155817    -2.054085     0.493252      51.15
 H      -2.876106    -2.213485    -0.529596      27.31
 C      -3.273190    -3.411411     1.239788      97.89
 O      -3.541222    -4.607814     0.322886     134.78
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 H      -3.106053    -4.365505    -0.657336      27.40
 H      -4.204134    -3.521456     1.821470      24.33
 H      -2.297069    -3.299976     1.626827      26.39
 C       1.004412    -2.021001     0.286478      59.91
 H       1.353623    -2.820294    -0.424657      23.85
 C       0.966301     0.276177     1.317768      64.36
 H       1.494055     1.117450     1.545560      18.73
 C      -0.532459     0.166513     1.329048      11.35
 O      -1.212916     1.352381     1.466504     127.85
 C      -0.523832     2.539268     2.299441      70.23
 H       0.154422     2.120602     3.140765      24.21
 H       0.264110     2.860280     1.313704      20.76
 H      -1.178088     3.341944     2.707178      25.04
 C      -1.068315    -1.029194     1.246679      27.23
 O      -2.538132    -1.106071     1.404366     189.82
 C      -0.428071    -2.094714     0.688149      43.88
 H      -1.060487    -2.989267     0.426901      22.09
 C       1.593850    -0.900140     0.689003      27.50
 C       3.156864    -0.803923     0.810945      92.46
 H       3.544620    -1.109876    -0.143351      26.69
 O       3.621811     0.651780     0.699852     193.18
 H       3.127100     0.988476     1.513496      25.88
 C       4.107302    -1.370930     1.933413      87.43
 H       3.806615    -0.790406     2.855425      26.31
 O       3.430401    -2.696913     2.393384     253.54
 H       3.727460    -3.521020     2.244717      33.67
 C       5.459173    -1.654327     1.622942      94.05
 O       6.558159    -0.590683     2.072175     190.63
 H       6.443432    -0.304747     3.064399      29.70
 H       5.552348    -1.867186     0.678474      31.56
 H       5.710354    -2.641363     2.215763      27.30
55
name= lig-ACN-Water-frame_1056
 C      -4.245821    -1.785387    -2.656769      29.58
 H      -3.997222    -2.822019    -2.684148      23.53
 C      -4.436362     0.534487    -1.751692      78.80
 H      -4.578122     1.330855    -0.880603      24.49
 C      -4.347893     1.017259    -3.100040      11.37
 O      -4.473526     2.274773    -3.570203     138.63
 C      -5.141996     3.129418    -2.518935      95.39
 H      -4.473842     3.595006    -1.696479      23.59
 H      -6.035526     2.472306    -2.562627      24.32
 H      -5.164414     4.191305    -3.080029      24.75
 C      -4.113775     0.127493    -4.144780      20.90
 O      -4.000808     0.618029    -5.446820     174.09
 H      -4.289013     1.580352    -5.486689      22.59
 C      -4.093628    -1.218388    -3.968661      36.84
 H      -3.582711    -1.894013    -4.763722      26.94
 C      -4.456127    -0.829594    -1.600572      32.49
 C      -4.730849    -1.470333    -0.209561      77.16
 H      -5.581759    -2.323981    -0.292348      24.22
 O      -5.362670    -0.432624     0.623528     204.21
 H      -4.697213     0.012545     1.296698      26.77
 C      -3.268579    -2.095591     0.340483      54.94
 H      -2.413813    -2.168803    -0.271531      27.26
 C      -3.385649    -3.482499     1.166462     114.60
 O      -3.526666    -4.518635     0.274540     213.02
 H      -3.043585    -4.415234    -0.610770      28.32
 H      -4.213624    -3.381603     2.007543      24.78
 H      -2.704931    -3.859309     1.913123      25.66
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 C       0.865208    -2.028529     0.233273      28.72
 H       1.513494    -2.916837    -0.177911      22.84
 C       0.914478     0.270425     1.186513      65.66
 H       1.426314     1.232041     1.211117      24.27
 C      -0.416187     0.249961     1.454526       6.58
 O      -1.282980     1.385946     1.576795     123.83
 C      -0.507733     2.530017     2.207083     100.51
 H      -0.032093     2.252929     3.155717      27.99
 H       0.174254     3.385204     1.475447      24.23
 H      -1.509303     3.036179     2.385639      25.43
 C      -1.181989    -1.068176     1.208292      -7.66
 O      -2.519248    -1.163253     1.351663     108.96
 C      -0.391169    -2.206368     0.596790      56.05
 H      -1.037109    -3.102086     0.214976      23.59
 C       1.736404    -0.835855     0.825554      13.13
 C       3.271469    -0.820898     0.693006      91.26
 H       3.578943    -1.390829    -0.107890      28.89
 O       3.653804     0.621850     0.684975     181.15
 H       3.646185     1.172918     1.477829      28.91
 C       3.984120    -1.452500     1.990465      79.37
 H       4.178846    -0.653571     2.711241      28.59
 O       3.396649    -2.694785     2.493928     240.88
 H       3.987323    -3.423351     2.127000      29.59
 C       5.574292    -1.730676     1.533252      66.65
 O       6.570724    -0.640529     2.073710     176.62
 H       6.155752    -0.462308     2.951921      30.34
 H       5.721952    -1.779511     0.539917      27.36
 H       5.886113    -2.719419     2.096164      28.26
55
name= lig-ACN-Water-frame_1057
 C      -4.227400    -1.761570    -2.676316      72.63
 H      -4.238593    -2.799548    -2.430795      26.69
 C      -4.582330     0.578168    -1.697875      42.80
 H      -4.893549     1.148712    -0.821837      24.14
 C      -4.366026     1.006228    -3.055615      26.37
 O      -4.546660     2.348870    -3.599271     157.50
 C      -5.203039     3.202558    -2.509528      98.28
 H      -4.476795     3.335337    -1.626183      24.42
 H      -5.998879     2.780679    -1.687635      24.84
 H      -5.840439     3.977693    -3.167112      23.25
 C      -4.092766     0.147835    -4.132616      25.79
 O      -4.072540     0.552790    -5.467300     163.13
 H      -4.448180     1.504183    -5.458036      26.72
 C      -3.992478    -1.247244    -3.946697      46.26
 H      -3.874256    -1.898880    -4.879548      17.80
 C      -4.376289    -0.892380    -1.525411     -25.55
 C      -4.635178    -1.452482    -0.140697      70.01
 H      -5.487854    -2.303383    -0.366731      22.88
 O      -5.288275    -0.339341     0.666648     208.39
 H      -4.893033    -0.395118     1.592723      27.13
 C      -3.333230    -2.136421     0.401239      79.15
 H      -3.016020    -2.332494    -0.607127      27.31
 C      -3.494302    -3.416075     1.159243     107.19
 O      -3.603098    -4.547995     0.153922     138.77
 H      -2.828503    -4.558545    -0.323470      32.10
 H      -4.638895    -3.431828     1.488422      23.17
 H      -2.625918    -3.387378     1.773480      26.32
 C       1.042824    -1.957211     0.380695      40.84
 H       1.609161    -2.868120    -0.096178      23.11
 C       0.963985     0.256389     1.100068      55.38
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 H       1.366762     1.331014     1.195671      21.68
 C      -0.498365     0.128618     1.440499      -0.32
 O      -1.178966     1.376126     1.685804     173.50
 C      -0.689571     2.589099     2.137277     109.33
 H      -0.023417     2.282306     2.979984      27.83
 H       0.246363     2.911441     1.315975      24.48
 H      -1.278900     3.463803     2.599846      25.06
 C      -1.175884    -1.066099     1.095802      12.41
 O      -2.613357    -1.165996     1.267458     148.65
 C      -0.463183    -2.174600     0.513435      50.22
 H      -0.605553    -3.271765     0.248157      23.20
 C       1.705294    -0.915903     0.778975      41.06
 C       3.264445    -0.757374     0.742232     101.76
 H       3.641295    -1.087650    -0.154108      27.50
 O       3.761214     0.567144     0.588860     226.21
 H       3.767533     0.798366     1.517369      29.53
 C       4.020893    -1.531134     1.928764      70.26
 H       3.906744    -0.832289     2.722770      27.01
 O       3.378003    -2.647733     2.567746     219.04
 H       4.009239    -3.591646     2.413574      25.15
 C       5.715002    -1.736454     1.551995      76.09
 O       6.475810    -0.755492     2.043117     280.12
 H       6.252756    -0.277924     2.831947      30.26
 H       5.806600    -1.701844     0.530663      26.92
 H       6.118457    -2.818325     1.787614      27.16
55
name= lig-ACN-Water-frame_1058
 C      -4.154593    -1.719077    -2.567706      41.06
 H      -4.287573    -2.781373    -2.425929      26.16
 C      -4.631618     0.472013    -1.814527      75.13
 H      -4.894439     1.041032    -1.050269      26.92
 C      -4.416997     1.066251    -3.071399      18.23
 O      -4.704639     2.393180    -3.432851     168.16
 C      -5.228924     3.304172    -2.518326     108.94
 H      -4.361466     4.053762    -2.208291      23.62
 H      -5.757140     2.474643    -1.823710      22.59
 H      -5.896571     4.205519    -2.899348      24.17
 C      -4.087571     0.092674    -4.155789       2.37
 O      -4.133655     0.542212    -5.494195     164.44
 H      -4.517291     1.398565    -5.495670      28.40
 C      -3.921385    -1.297255    -3.916856      50.59
 H      -4.083761    -1.968491    -4.754677      17.83
 C      -4.420095    -0.828283    -1.506392      47.11
 C      -4.631314    -1.338198    -0.084196      93.94
 H      -5.379219    -2.284049     0.048903      23.66
 O      -5.161315    -0.358823     0.728862     295.52
 H      -4.964175    -0.528770     1.625022      30.56
 C      -3.391210    -2.059210     0.403612      95.12
 H      -2.627097    -2.378182    -0.308301      24.98
 C      -3.655629    -3.433207     1.096801     104.63
 O      -3.657573    -4.549056     0.117327     132.15
 H      -2.868200    -4.726938    -0.485152      26.67
 H      -4.574687    -3.623826     1.881618      23.47
 H      -3.010295    -3.682461     1.926732      24.95
 C       1.060712    -2.130406     0.499553      51.13
 H       1.627227    -3.012388     0.070224      23.39
 C       0.871431     0.251082     1.170976      53.98
 H       1.542096     1.186507     1.414281      17.48
 C      -0.466265     0.162254     1.275294      18.60
 O      -1.231412     1.197660     1.729063     126.12
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 C      -0.574527     2.620496     2.159674      86.90
 H       0.050599     2.702419     3.043741      26.15
 H      -0.176791     3.132243     1.092893      23.90
 H      -1.663238     3.077424     2.104230      23.49
 C      -1.228683    -1.097024     0.951874       5.17
 O      -2.642144    -1.127335     1.144794     175.68
 C      -0.294100    -2.073771     0.461475      68.87
 H      -1.059016    -2.844280     0.280917      22.63
 C       1.753858    -0.779893     0.745198      26.16
 C       3.268484    -0.867888     0.677984      75.22
 H       3.393012    -1.466676    -0.200820      23.44
 O       3.881277     0.535150     0.580437     222.95
 H       3.647774     1.300138     1.225480      24.11
 C       4.196917    -1.524117     1.900476      65.91
 H       4.320128    -0.752399     2.560375      23.92
 O       3.377777    -2.654162     2.577275     250.77
 H       3.670222    -3.620246     2.734523      28.86
 C       5.557221    -1.826229     1.503439      92.02
 O       6.503982    -0.708454     2.071645     204.14
 H       6.171615    -0.672073     3.016587      30.54
 H       5.714093    -1.807658     0.488164      29.64
 H       5.832424    -2.830825     1.988711      27.13
55
name= lig-ACN-Water-frame_1059
 C      -4.072266    -1.775162    -2.503204      53.60
 H      -3.806768    -2.842893    -2.345281      23.87
 C      -4.657257     0.543355    -1.828503      67.25
 H      -4.858010     1.225218    -1.159188      25.87
 C      -4.484626     1.021195    -3.202796      12.24
 O      -4.806013     2.357787    -3.435224     108.73
 C      -5.246961     3.462841    -2.425351      84.33
 H      -4.416946     4.187932    -2.060686      24.13
 H      -5.691023     3.321111    -1.247542      22.27
 H      -6.117617     3.634438    -3.140521      22.79
 C      -4.135055     0.139662    -4.181148      34.13
 O      -4.170671     0.530779    -5.520316     169.32
 H      -4.563105     1.445270    -5.524004      22.22
 C      -3.975174    -1.247924    -3.828458      48.06
 H      -3.607696    -1.961580    -4.516146      29.64
 C      -4.505096    -0.839993    -1.537631      19.97
 C      -4.714836    -1.395156    -0.111394      66.49
 H      -5.654617    -2.039536    -0.445086      24.21
 O      -5.061516    -0.309084     0.830570     236.57
 H      -4.714231    -0.398908     1.803175      26.11
 C      -3.330297    -2.084799     0.372688      46.64
 H      -2.950485    -2.347614    -0.641636      27.05
 C      -3.704638    -3.545644     1.146457      98.57
 O      -3.737073    -4.513485     0.107758     110.77
 H      -2.945778    -4.251535    -0.593018      25.65
 H      -4.855476    -3.328607     1.344907      22.47
 H      -2.895468    -3.745737     1.831676      27.19
 C       1.103692    -2.089904     0.542126      36.32
 H       1.677340    -2.971765     0.427288      23.88
 C       0.973729     0.242989     1.214550      81.16
 H       1.160400     1.244449     1.738580      19.28
 C      -0.506476     0.227357     1.150953      10.84
 O      -1.274807     1.138235     1.823431     158.79
 C      -0.639182     2.559458     2.027466      89.91
 H       0.037835     2.556337     2.901010      26.12
 H       0.075181     2.975541     1.107373      24.62
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 H      -1.549319     3.145542     2.515569      24.16
 C      -1.148107    -0.987127     0.831020      14.56
 O      -2.508581    -1.021649     1.089294     130.19
 C      -0.381358    -2.157501     0.464276      66.81
 H      -0.471656    -3.060665    -0.048008      23.42
 C       1.752706    -0.925826     0.796713      29.58
 C       3.345531    -0.834451     0.707322      91.35
 H       3.802329    -1.322322    -0.170509      24.04
 O       3.975346     0.436373     0.514730     229.02
 H       3.259879     0.976565     0.952352      27.38
 C       4.029844    -1.512802     1.939592      87.73
 H       4.115344    -0.821729     2.659385      29.31
 O       3.388257    -2.596535     2.561808     313.45
 H       4.023165    -3.179373     2.458294      34.61
 C       5.598899    -1.864996     1.495479      79.31
 O       6.499356    -0.772767     2.049448     208.95
 H       6.327179    -0.512213     3.043940      29.31
 H       5.842717    -1.990500     0.434785      27.56
 H       5.945371    -2.830408     1.964302      27.89
55
name= lig-ACN-Water-frame_1060
 C      -4.052871    -1.692569    -2.535710      66.29
 H      -3.622290    -2.683743    -2.230752      23.83
 C      -4.675221     0.568237    -1.828050      82.30
 H      -4.959465     1.134196    -0.987806      24.67
 C      -4.618650     1.035059    -3.084217      -1.11
 O      -4.857365     2.358136    -3.471189      88.44
 C      -5.314016     3.558409    -2.392546      84.59
 H      -4.461304     4.155540    -2.807652      25.38
 H      -5.419184     3.118845    -1.214741      22.98
 H      -6.158148     4.207504    -2.737514      27.02
 C      -4.250964     0.108133    -4.217530       4.00
 O      -4.175178     0.514917    -5.579471      96.27
 H      -4.537306     1.478705    -5.603419      19.55
 C      -3.923324    -1.231612    -3.832166      60.71
 H      -3.398275    -1.676460    -4.618159      25.09
 C      -4.536982    -0.825082    -1.497880      25.40
 C      -4.723657    -1.351166    -0.081557      78.75
 H      -5.406487    -2.218505     0.279292      24.75
 O      -5.040888    -0.295936     0.849750     292.96
 H      -4.216545    -0.341110     1.432530      27.39
 C      -3.360209    -2.169495     0.353771      63.36
 H      -2.648809    -2.414933    -0.479916      24.23
 C      -3.648835    -3.400289     1.118349     107.25
 O      -3.788401    -4.461773     0.042906     131.08
 H      -3.018599    -4.539819    -0.640079      27.30
 H      -4.690558    -3.480851     1.711448      24.30
 H      -3.152394    -3.687759     2.048350      26.00
 C       1.065762    -2.046426     0.533293      50.73
 H       1.568675    -2.896364     0.230839      25.66
 C       1.023259     0.223854     1.221219      73.88
 H       1.779907     0.923432     1.552639      23.18
 C      -0.380742     0.230331     1.164778     -18.18
 O      -1.291862     1.204439     1.865996     147.29
 C      -0.720075     2.428333     2.016096     115.78
 H       0.238467     2.325596     2.574266      26.79
 H      -0.423010     2.630893     0.808029      26.51
 H      -1.261236     3.398425     2.175091      26.39
 C      -1.087701    -1.057793     0.678219     -24.89
 O      -2.452343    -1.006651     0.979298      95.08
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 C      -0.339200    -2.246886     0.452216      63.61
 H      -0.998501    -2.997976     0.306924      22.58
 C       1.804266    -0.858661     0.898004      28.06
 C       3.361467    -0.897957     0.707944      89.08
 H       3.366818    -1.629701    -0.166581      25.05
 O       3.969521     0.395402     0.461387     220.28
 H       3.625196     1.217196     0.765149      30.89
 C       4.011769    -1.409344     1.996780      84.55
 H       3.907276    -0.611496     2.612312      30.82
 O       3.391922    -2.617057     2.524033     234.20
 H       3.892667    -3.538707     2.517556      27.82
 C       5.652862    -1.821294     1.632678      82.86
 O       6.520856    -0.878208     1.995655     283.00
 H       6.085221    -0.491802     2.774755      30.21
 H       5.656949    -1.788018     0.554180      26.88
 H       5.841490    -2.842025     2.032042      28.42
55
name= lig-ACN-Water-frame_1061
 C      -4.044230    -1.585910    -2.554887      29.81
 H      -3.878445    -2.692359    -2.432753      25.54
 C      -4.777406     0.496511    -1.684555      48.56
 H      -5.114420     1.243669    -0.879051      24.29
 C      -4.756464     1.063201    -3.124149       2.87
 O      -4.988195     2.454017    -3.482977     131.97
 C      -5.235992     3.532862    -2.532296     128.71
 H      -4.516428     4.378190    -2.499704      27.14
 H      -4.828508     3.097404    -1.457078      25.27
 H      -6.361188     3.721392    -2.523056      26.77
 C      -4.389233     0.144889    -4.172603      19.55
 O      -4.179777     0.502552    -5.555187     205.91
 H      -4.504975     1.371725    -5.710126      31.95
 C      -3.823475    -1.133117    -3.940197      53.70
 H      -3.609924    -1.948208    -4.600559      20.13
 C      -4.534551    -0.836125    -1.493325      42.11
 C      -4.608354    -1.369793    -0.028817      98.19
 H      -5.584010    -1.984528    -0.251884      25.50
 O      -5.023223    -0.348373     0.842198     292.68
 H      -4.461853     0.341944     1.137507      30.10
 C      -3.302528    -2.028588     0.318607      89.71
 H      -2.920136    -2.516673    -0.654006      28.63
 C      -3.605894    -3.377903     1.126877     109.71
 O      -3.832518    -4.394263     0.030568     126.38
 H      -3.006014    -4.734013    -0.143859      32.11
 H      -4.627822    -3.255014     1.625414      25.92
 H      -2.618721    -3.640506     1.517810      27.00
 C       1.098778    -2.155690     0.440762      39.19
 H       1.814884    -2.853859     0.031218      24.02
 C       1.083577     0.326764     1.286051      63.06
 H       1.291709     1.309035     1.500967      22.54
 C      -0.401490     0.142548     1.274161       3.45
 O      -1.310567     1.054985     1.804063     101.47
 C      -0.609495     2.479802     1.878425      96.70
 H       0.186008     2.708430     2.619309      27.34
 H      -0.328597     2.970634     0.758012      26.75
 H      -1.502826     2.734777     2.413276      26.78
 C      -1.052607    -0.982850     0.760606      30.45
 O      -2.457952    -1.071111     0.847140     162.63
 C      -0.315298    -2.146922     0.457212      64.33
 H      -0.530701    -3.130571     0.526521      25.88
 C       1.764863    -0.917101     0.855302      19.01
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 C       3.226559    -0.937873     0.746939      71.29
 H       3.733734    -1.556911    -0.097423      25.37
 O       3.986003     0.370627     0.342269     157.38
 H       3.480999     0.922585     1.008851      29.88
 C       4.153312    -1.470672     2.044962      97.10
 H       4.214005    -0.831310     2.840005      29.41
 O       3.330567    -2.633629     2.516342     166.23
 H       4.038205    -3.465407     2.333900      27.61
 C       5.456611    -1.835480     1.670197      93.89
 O       6.636930    -0.848139     2.056093     252.54
 H       6.542589    -0.448329     2.941591      31.77
 H       5.610735    -2.187459     0.629562      27.29
 H       5.702170    -2.744931     2.181464      28.62
55
name= lig-ACN-Water-frame_1062
 C      -4.012693    -1.605663    -2.641063      74.50
 H      -3.838666    -2.677165    -2.488488      25.06
 C      -4.946544     0.601290    -1.808520      81.63
 H      -5.255923     1.224028    -0.804253      24.30
 C      -4.866365     1.085364    -3.089277       0.65
 O      -5.071556     2.445087    -3.576545     168.20
 C      -5.140909     3.422155    -2.526962     116.99
 H      -4.979052     4.346223    -3.133183      25.62
 H      -4.646806     3.209869    -1.449379      24.68
 H      -6.244291     3.562524    -2.303806      26.43
 C      -4.379506     0.254667    -4.179396      18.64
 O      -4.225099     0.537216    -5.494479     142.84
 H      -4.643794     1.409673    -5.692884      27.40
 C      -3.925742    -1.049928    -3.845932      38.20
 H      -3.661181    -1.536177    -4.806331      18.94
 C      -4.451379    -0.746291    -1.535326      -8.63
 C      -4.576783    -1.317164    -0.150969      84.63
 H      -5.243330    -2.271968     0.029127      24.31
 O      -5.115753    -0.417673     0.867415     230.58
 H      -4.422678     0.333579     0.816943      27.95
 C      -3.252657    -2.085670     0.217087      77.35
 H      -2.719762    -2.321502    -0.790374      27.12
 C      -3.467858    -3.344595     1.044118     130.67
 O      -3.901132    -4.347215     0.104851     167.72
 H      -3.070630    -4.861772    -0.261027      26.04
 H      -4.122505    -3.310975     1.936811      27.95
 H      -2.648848    -3.712200     1.722057      26.70
 C       1.197437    -2.042958     0.372563      56.46
 H       1.578745    -3.112914     0.159747      21.91
 C       0.963139     0.198266     1.266691      90.25
 H       1.589646     0.959882     1.520563      23.73
 C      -0.385317     0.045203     1.373057      24.77
 O      -1.193755     1.069664     1.712918     173.63
 C      -0.720352     2.528179     1.858093      97.78
 H       0.222022     2.250863     2.448778      24.03
 H      -0.485643     3.019828     0.752870      26.02
 H      -1.388490     3.276774     2.229672      27.08
 C      -1.055640    -1.126690     0.902281       9.03
 O      -2.431274    -0.996584     0.817726     151.22
 C      -0.248192    -2.180039     0.465553      74.57
 H      -0.904235    -2.832414    -0.036076      24.64
 C       1.762152    -0.858278     0.777648      40.16
 C       3.413398    -0.887599     0.802369      74.04
 H       3.443545    -1.758550    -0.006804      24.76
 O       3.878579     0.314912     0.289190     249.65
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H	3.976495	1.112128	0.923050	27.13
C	3.950966	-1.483124	2.083984	87.89
H	4.014661	-0.770532	2.852186	27.34
O	3.320566	-2.662610	2.518004	313.50
H	3.763530	-3.471428	2.431455	31.53
C	5.649761	-1.885847	1.751886	75.81
O	6.650605	-0.867946	2.073210	246.59
H	6.548588	-0.810982	3.080047	30.03
H	5.836433	-2.003676	0.627047	27.11
H	5.788956	-2.709296	2.361479	29.06