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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 3

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

55
name = lig-etoh-frame_1

C	2.861244	1.713103	-1.715484	45.15
H	2.584566	2.269491	-2.582777	21.02
C	3.278344	0.892826	0.515182	34.38
H	3.098900	0.788749	1.542990	21.01
C	3.840293	-0.443515	0.212306	6.85
O	4.368579	-1.243990	1.200663	197.35
C	5.732663	-1.900978	1.005220	96.40
H	5.730795	-2.863960	0.412494	25.03
H	6.164596	-1.992544	1.948227	27.62
H	6.369202	-1.149411	0.334774	26.31
C	4.042396	-0.504391	-1.140001	12.38
O	4.547075	-1.723551	-1.682676	201.42
H	4.035046	-2.195439	-2.490106	23.78
C	3.445050	0.444365	-2.114557	53.78
H	4.005434	0.319665	-3.036080	25.46
C	2.682757	1.819878	-0.369722	43.72
C	1.869977	3.047995	0.253604	129.00
H	2.221887	3.842095	-0.263871	23.31
O	2.235359	3.365747	1.550351	287.04
H	3.154987	3.834747	1.473799	28.89
C	0.320304	2.899290	0.180249	79.61
H	0.118917	2.701618	-0.893750	22.63
C	-0.161149	4.403845	0.685139	96.45
O	0.609664	5.513059	-0.167905	256.33
H	0.585987	5.273425	-1.052226	31.65
H	0.394820	4.335261	1.565835	25.94
H	-1.207487	4.465730	0.681458	27.18
C	-0.969840	-1.414986	-0.591995	44.59
H	-0.236869	-2.235491	-0.707250	20.13
C	-2.923567	0.022662	-0.684844	35.54
H	-4.082246	0.076730	-0.892291	20.66
C	-2.262921	1.050927	-0.111206	29.04
O	-2.873373	2.374317	-0.193896	237.78
C	-3.503780	2.708833	1.123023	121.30
H	-4.030531	1.858732	1.655221	27.24
H	-2.842599	3.085582	1.768383	29.38
H	-4.032873	3.626194	1.160273	28.02
C	-1.086400	0.861367	0.395591	9.52

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 O      -0.219713     1.894904     0.950487     233.36
 C      -0.320005    -0.276995     0.064140      37.54
 H       0.675969    -0.228778     0.466029      18.45
 C      -2.254982    -1.248039    -0.980133      29.10
 C      -3.081250    -2.362668    -1.496893      87.56
 H      -4.033368    -1.878509    -1.714849      25.22
 O      -2.594662    -2.881866    -2.769135     279.59
 H      -2.849436    -3.872261    -2.685068      20.28
 C      -3.400662    -3.421733    -0.262203     100.90
 H      -2.430763    -3.666117     0.020940      26.19
 O      -4.034919    -2.900723     0.826980     363.77
 H      -3.392202    -2.595164     1.383375      31.33
 C      -4.304520    -4.604345    -0.726105      89.32
 O      -3.658306    -5.438323    -1.857242     268.67
 H      -3.086978    -5.964686    -1.004327      21.35
 H      -5.253875    -4.132902    -1.015986      26.28
 H      -4.482817    -5.345772     0.103468      26.39
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name = lig-etoh-frame_2
 C       2.835965     1.679072    -1.787809      26.06
 H       2.594053     2.572354    -2.502087      19.00
 C       3.244733     0.856293     0.549208      24.56
 H       3.082642     0.838552     1.694591      18.21
 C       3.850040    -0.448234     0.120166      16.36
 O       4.401991    -1.249953     1.157600     217.14
 C       5.720300    -1.894990     0.986059     102.40
 H       5.550729    -2.819286     0.416074      24.74
 H       6.424560    -1.903286     1.938646      25.23
 H       6.341771    -1.170108     0.393720      27.15
 C       4.037437    -0.605524    -1.192339      28.56
 O       4.587159    -1.748478    -1.677962     202.83
 H       4.037369    -1.799666    -2.570488      22.96
 C       3.439818     0.474792    -2.125349      58.54
 H       3.719326     0.306599    -3.223624      25.91
 C       2.742696     1.871265    -0.290554      74.36
 C       1.819332     2.953318     0.229235     120.22
 H       1.922417     3.892711    -0.619684      16.73
 O       2.232673     3.377280     1.575845     262.96
 H       3.231801     3.685721     1.459552      28.75
 C       0.267377     2.956032     0.079187      59.42
 H       0.018588     2.672140    -0.953247      19.89
 C      -0.161676     4.452731     0.660436      84.46
 O       0.608732     5.530197    -0.124096     180.04
 H       0.472694     5.179724    -1.177060      24.18
 H       0.414500     4.396458     1.646681      23.33
 H      -1.330619     4.584685     0.638946      23.47
 C      -0.893441    -1.395016    -0.569372      60.40
 H      -0.165147    -2.113846    -1.004986      20.50
 C      -3.015655    -0.085601    -0.763146      24.18
 H      -4.040801     0.170400    -0.816750      21.25
 C      -2.301728     1.044540    -0.164321      -3.81
 O      -2.905001     2.375000    -0.164712     218.86
 C      -3.411469     2.735963     1.081764     106.12
 H      -4.228344     2.030253     1.477631      25.03
 H      -2.685931     3.052577     2.062047      23.02
 H      -4.330858     3.537642     0.832446      23.85
 C      -1.043700     0.853672     0.407356      11.75
 O      -0.229531     1.910402     0.933916     191.48
 C      -0.403801    -0.298183     0.025718      26.94
 H       0.843014    -0.285209     0.429682      14.81
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 C      -2.229771    -1.318383    -1.000835      25.56
 C      -3.074976    -2.300957    -1.446342      79.99
 H      -4.108018    -1.954798    -1.721604      23.49
 O      -2.617290    -2.918371    -2.728319     272.66
 H      -2.913917    -3.799744    -2.619206      25.39
 C      -3.337165    -3.416743    -0.243305      68.65
 H      -2.227285    -3.923459    -0.180378      21.78
 O      -4.128407    -2.895981     0.806985     284.20
 H      -3.532412    -2.451424     1.559795      24.97
 C      -4.242742    -4.604262    -0.753586      83.63
 O      -3.633824    -5.436691    -1.801039     318.29
 H      -3.212464    -6.045288    -1.211385      29.41
 H      -5.293620    -4.222816    -0.945272      27.11
 H      -4.380420    -5.089686     0.263974      26.30
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name = lig-etoh-frame_3
 C       2.833352     1.642629    -1.791366      74.05
 H       2.613697     2.514881    -2.299583      27.20
 C       3.210283     0.778837     0.606546      31.73
 H       3.083709     1.069784     1.611219      20.98
 C       3.877344    -0.376466     0.110649       6.34
 O       4.426654    -1.255695     1.127151     203.51
 C       5.710007    -1.857465     0.949725     115.05
 H       5.529708    -2.857048     0.525322      25.50
 H       6.224581    -1.967982     1.902401      27.16
 H       6.377804    -1.222790     0.271204      26.79
 C       3.973844    -0.644550    -1.316404      16.93
 O       4.621354    -1.780393    -1.713527     238.48
 H       4.340569    -1.727856    -2.575696      29.99
 C       3.485313     0.463657    -2.161181      52.57
 H       3.269295     0.277573    -3.263259      20.49
 C       2.769336     1.880880    -0.243599      25.64
 C       1.802137     2.925930     0.158561     116.50
 H       1.867909     3.653977    -0.547092      21.81
 O       2.236305     3.387470     1.588856     269.92
 H       3.170306     3.498102     1.600443      29.73
 C       0.236516     3.021256     0.002706      44.18
 H      -0.098467     2.801722    -1.057717      20.23
 C      -0.123921     4.478752     0.603813     106.70
 O       0.572998     5.514801    -0.084375     284.87
 H       0.427968     5.457857    -1.032026      31.31
 H       0.064547     4.644235     1.679403      24.88
 H      -1.137690     4.704157     0.623596      25.71
 C      -0.823178    -1.400795    -0.599953      58.50
 H      -0.248694    -2.096816    -1.151761      20.39
 C      -3.025395    -0.150334    -0.802689      37.41
 H      -4.139130     0.018963    -1.000058      19.48
 C      -2.395052     1.050652    -0.225804     -20.15
 O      -2.915391     2.338535    -0.148632     232.17
 C      -3.410105     2.806582     1.097819     118.79
 H      -4.159285     1.970942     1.334371      25.49
 H      -2.720221     2.899634     1.820488      27.64
 H      -4.033525     3.470838     0.598162      24.84
 C      -0.966111     0.901450     0.393175      -6.78
 O      -0.271823     1.905807     0.945323     184.50
 C      -0.372002    -0.309822     0.055016      37.38
 H       0.608035    -0.356137     0.207226      20.02
 C      -2.240310    -1.266939    -0.984809      27.67
 C      -3.148285    -2.352227    -1.431602      73.79
 H      -4.177230    -1.960970    -1.627976      24.03
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 O      -2.631684    -2.961109    -2.670647     239.32
 H      -2.995735    -3.954551    -2.705626      19.83
 C      -3.253350    -3.435657    -0.309624      89.79
 H      -2.405891    -3.938404    -0.003610      24.43
 O      -4.193841    -2.879101     0.805399     269.38
 H      -3.730866    -2.411615     1.599827      25.43
 C      -4.189387    -4.582036    -0.740239     101.32
 O      -3.623457    -5.431070    -1.732643     292.77
 H      -3.118077    -6.291090    -1.392356      27.99
 H      -5.173703    -4.345329    -1.133111      27.29
 H      -4.282891    -5.093711     0.201628      27.59
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name = lig-etoh-frame_4
 C       2.867242     1.603480    -1.650241      53.89
 H       2.537207     2.425880    -2.446259      23.01
 C       3.171517     0.750460     0.628300      43.69
 H       3.153662     1.060466     1.716596      20.37
 C       3.926240    -0.311428     0.116931       8.08
 O       4.425074    -1.236819     1.091708     193.81
 C       5.694590    -1.830551     0.894342     112.72
 H       5.650140    -2.925590     0.600696      25.82
 H       6.017833    -1.965511     1.992837      25.46
 H       6.468248    -1.385264     0.117083      25.97
 C       3.887149    -0.602810    -1.376403       5.12
 O       4.642025    -1.809821    -1.768256     123.75
 H       4.840916    -1.969321    -2.865586      24.84
 C       3.504553     0.415801    -2.243178      52.58
 H       3.186752     0.192744    -3.232882      20.87
 C       2.763208     1.792551    -0.285970      34.46
 C       1.817544     2.943733     0.127445     102.16
 H       2.260330     3.887044    -0.605177      19.79
 O       2.206921     3.390060     1.574842     243.54
 H       3.287503     3.364332     1.664689      25.94
 C       0.233929     3.055335     0.008622      59.54
 H      -0.092013     2.949130    -0.990274      21.42
 C      -0.101357     4.489071     0.550300     106.06
 O       0.547704     5.522305    -0.041194     255.87
 H       0.392876     5.622402    -1.049396      28.54
 H      -0.032203     4.652663     1.636182      25.17
 H      -1.280657     4.672983     0.391207      22.99
 C      -0.866430    -1.407225    -0.682973      43.05
 H      -0.216453    -2.247702    -1.128385      18.99
 C      -3.013338    -0.089118    -0.794151      57.71
 H      -3.988990    -0.330945    -1.285860      20.47
 C      -2.407724     1.034157    -0.236403      11.71
 O      -2.906866     2.279618    -0.180644     222.48
 C      -3.475821     2.822736     1.080866      81.55
 H      -4.067245     1.990786     1.516398      24.11
 H      -2.528764     3.012270     1.884464      21.88
 H      -3.848895     3.981589     0.755474      22.68
 C      -1.003318     0.934206     0.301967      12.24
 O      -0.319599     1.933463     0.963169     180.50
 C      -0.287152    -0.302906     0.109371       8.74
 H       1.053598    -0.368087     0.146020      15.34
 C      -2.252843    -1.232611    -0.970313      18.90
 C      -3.201478    -2.456360    -1.427405      68.92
 H      -4.218905    -2.027427    -1.528911      24.21
 O      -2.649917    -3.022503    -2.615339     275.68
 H      -2.991560    -3.915459    -2.789081      22.20
 C      -3.255422    -3.439325    -0.365345      90.76
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 H      -2.335490    -3.796087     0.328599      19.51
 O      -4.234353    -2.864251     0.791093     266.31
 H      -3.727029    -2.493464     1.452507      28.28
 C      -4.136510    -4.585252    -0.698328      94.71
 O      -3.601455    -5.441924    -1.695417     271.65
 H      -3.058657    -6.379173    -1.418251      25.79
 H      -5.063512    -4.270277    -1.277707      25.00
 H      -4.363625    -5.288258     0.196504      24.09
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name = lig-etoh-frame_5
 C       2.930542     1.553729    -1.587133      56.34
 H       2.483267     2.112972    -2.308630      25.19
 C       3.156799     0.763203     0.635091      48.33
 H       3.213367     0.791999     1.716662      22.47
 C       3.964764    -0.289805     0.101482      11.29
 O       4.402451    -1.193094     1.029536     199.78
 C       5.705600    -1.862154     0.860898     117.58
 H       5.613203    -2.890524     0.553158      27.34
 H       6.056002    -1.767276     1.935656      26.51
 H       6.393929    -1.421802     0.205949      29.40
 C       3.870499    -0.582064    -1.395721      11.16
 O       4.639604    -1.824836    -1.834676     200.78
 H       5.195359    -1.960744    -2.623836      28.32
 C       3.469000     0.388145    -2.290550      37.62
 H       3.354514     0.160135    -3.443856      19.01
 C       2.691036     1.687628    -0.307425      42.18
 C       1.904417     3.031931     0.113047     115.40
 H       2.350894     3.765677    -0.362013      25.34
 O       2.178980     3.375019     1.541584     318.93
 H       3.138655     3.380485     1.568834      29.39
 C       0.288286     3.065710     0.081150      67.91
 H      -0.088119     2.948955    -1.006863      20.14
 C      -0.182175     4.474171     0.516653     109.53
 O       0.558564     5.580670    -0.018582     250.82
 H       0.381946     5.555213    -1.097672      26.27
 H       0.062305     4.452875     1.623042      25.20
 H      -1.164564     4.416413     0.260994      26.25
 C      -0.916383    -1.365671    -0.736651      34.15
 H      -0.380304    -2.259220    -0.890832      20.66
 C      -2.998122    -0.028473    -0.794162      44.94
 H      -3.897589    -0.161724    -1.336829      22.17
 C      -2.348223     1.020878    -0.197139      26.55
 O      -2.930841     2.263065    -0.225608     235.83
 C      -3.490539     2.860300     1.062372     115.68
 H      -4.206714     2.269226     1.770408      25.22
 H      -2.663027     3.039912     1.665238      26.33
 H      -3.709812     3.853453     1.171562      27.66
 C      -1.046235     0.898877     0.189118      -8.89
 O      -0.372473     2.001072     0.959737     187.93
 C      -0.168295    -0.316539     0.099793       5.04
 H       0.764741    -0.259782     0.279816      18.50
 C      -2.275127    -1.274868    -0.979390      15.42
 C      -3.185486    -2.501373    -1.429688      69.97
 H      -4.281830    -2.171964    -1.557421      23.69
 O      -2.660387    -3.080894    -2.588382     281.67
 H      -3.035852    -3.959684    -2.739376      22.12
 C      -3.300549    -3.464483    -0.280941     108.52
 H      -2.382368    -3.480658     0.199249      24.42
 O      -4.261348    -2.853234     0.744742     286.01
 H      -3.490709    -2.529704     1.423638      23.47
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 C      -4.117631    -4.656920    -0.656669     101.66
 O      -3.554647    -5.488858    -1.708162     366.35
 H      -3.144460    -6.069153    -1.167181      30.54
 H      -4.963519    -4.101533    -1.075389      27.67
 H      -4.503618    -5.187408     0.151374      26.72
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name = lig-etoh-frame_6
 C       2.986586     1.468108    -1.675193      64.82
 H       2.318175     2.244231    -2.291775      14.88
 C       3.192062     0.745025     0.628045      37.29
 H       3.122877     0.674142     1.720719      20.43
 C       3.955950    -0.290430     0.032655       6.00
 O       4.391378    -1.160432     0.963805     195.46
 C       5.703969    -1.896598     0.868246      96.12
 H       5.460751    -2.948949     0.488543      24.20
 H       6.242494    -1.733007     1.810180      26.45
 H       6.408628    -1.195904     0.114984      25.80
 C       3.956322    -0.612821    -1.402596      14.51
 O       4.608477    -1.822962    -1.854125     209.54
 H       5.299912    -1.644925    -2.523780      23.97
 C       3.417631     0.362921    -2.308406      51.32
 H       3.609912     0.339825    -3.320697      28.29
 C       2.571267     1.649759    -0.234447      65.69
 C       1.972946     3.061393     0.162554      98.79
 H       2.447328     4.017462    -0.561995      23.65
 O       2.156574     3.348010     1.503469     288.01
 H       3.144966     3.515142     1.584478      29.84
 C       0.371578     3.056398     0.113229      86.41
 H       0.072001     2.822148    -0.864009      22.44
 C      -0.229833     4.426207     0.533888      94.76
 O       0.562802     5.643617    -0.026621     234.21
 H       0.507702     5.495959    -0.923773      32.32
 H      -0.033714     4.412395     1.575945      27.40
 H      -1.421807     4.310550     0.401783      23.60
 C      -0.906981    -1.300916    -0.713212      41.54
 H      -0.526304    -2.377479    -0.734415      19.65
 C      -2.967627    -0.049680    -0.819584      24.02
 H      -4.031373     0.396460    -1.203374      22.26
 C      -2.314108     1.032086    -0.161577       6.80
 O      -2.999721     2.296669    -0.255406     170.76
 C      -3.469130     2.864223     1.076413      90.75
 H      -4.291908     2.435445     1.613487      25.59
 H      -2.434504     2.845547     1.738983      21.43
 H      -3.929011     4.011461     1.004268      24.22
 C      -0.949526     0.847609     0.146004       6.00
 O      -0.428708     2.072683     0.923719     158.46
 C      -0.218271    -0.315024    -0.005025      27.42
 H       0.990458    -0.200100     0.592086      12.95
 C      -2.340434    -1.308083    -1.006173      17.20
 C      -3.160782    -2.492725    -1.422348      72.42
 H      -4.184078    -2.194736    -1.681586      23.46
 O      -2.650651    -3.139395    -2.596023     246.88
 H      -3.087391    -4.107216    -2.591012      17.27
 C      -3.367093    -3.473693    -0.149858      91.10
 H      -2.215919    -3.515223     0.182946      20.19
 O      -4.244382    -2.833819     0.703070     336.50
 H      -3.627875    -2.565129     1.447174      26.37
 C      -4.131175    -4.716863    -0.648006      77.68
 O      -3.517168    -5.538795    -1.721837     306.50
 H      -2.938701    -6.074885    -0.837160      18.94
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 H      -5.041727    -4.104076    -0.944961      26.72
 H      -4.594429    -5.256381     0.299853      25.74
55
name = lig-etoh-frame_7
 C       2.911096     1.474692    -1.739974      43.28
 H       2.544901     2.295146    -2.287218      17.20
 C       3.222623     0.728083     0.605951      35.52
 H       3.014279     0.692518     1.700703      18.34
 C       3.927164    -0.324014    -0.076284      10.72
 O       4.412850    -1.167215     0.935885     220.03
 C       5.688565    -1.877250     0.835538     118.78
 H       5.502213    -2.863095     0.524787      27.56
 H       6.338195    -1.903444     1.818864      26.47
 H       6.219525    -1.421321     0.140593      30.27
 C       4.067720    -0.643913    -1.399186      28.30
 O       4.567427    -1.812536    -1.861750     189.78
 H       5.315023    -1.224414    -2.417601      20.37
 C       3.414590     0.298292    -2.292178      36.71
 H       3.816803     0.468847    -3.405064      25.57
 C       2.509706     1.647779    -0.214863      39.28
 C       2.002101     3.062803     0.187047     111.32
 H       2.239387     3.723596    -0.503863      25.99
 O       2.179172     3.330121     1.501657     279.07
 H       3.131645     3.721564     1.762365      27.97
 C       0.438584     3.048556     0.097418      67.81
 H       0.242677     2.732821    -1.001848      19.42
 C      -0.254962     4.379434     0.566139      87.20
 O       0.533721     5.676571    -0.011605     172.06
 H       0.656375     5.455051    -1.099857      25.70
 H      -0.147097     4.573673     1.710501      24.53
 H      -1.280974     4.492603     0.491259      25.81
 C      -0.923884    -1.322086    -0.668839      37.24
 H      -0.539233    -2.315171    -0.668798      21.08
 C      -2.974092    -0.032686    -0.843230      40.18
 H      -3.861376     0.446716    -0.957667      26.12
 C      -2.293390     1.038637    -0.170329     -12.16
 O      -3.078519     2.329292    -0.259225     149.24
 C      -3.416390     2.909278     1.100994     102.34
 H      -4.373117     2.240817     1.329051      23.79
 H      -2.601670     2.684136     1.781550      23.91
 H      -3.768881     3.743959     0.607009      25.12
 C      -0.848570     0.907837     0.170149       4.66
 O      -0.462405     2.113283     0.873602     203.54
 C      -0.236617    -0.287879    -0.091478      52.07
 H       0.545601    -0.440546     0.372297      21.05
 C      -2.378773    -1.282879    -1.035010      21.69
 C      -3.148868    -2.491690    -1.412333      69.13
 H      -4.161582    -2.058930    -1.763030      21.36
 O      -2.628942    -3.212465    -2.612277     268.53
 H      -2.917170    -4.096088    -2.477086      20.59
 C      -3.365092    -3.481153    -0.093068      97.77
 H      -2.444806    -3.853119     0.325585      21.88
 O      -4.226264    -2.798009     0.707411     354.50
 H      -3.886985    -2.533256     1.540935      30.15
 C      -4.196229    -4.745746    -0.622029     101.48
 O      -3.473311    -5.602937    -1.657684     348.85
 H      -2.819618    -6.113008    -1.251008      31.02
 H      -5.129982    -4.423094    -1.089309      27.06
 H      -4.385724    -5.408809     0.168069      27.97
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name = lig-etoh-frame_8
 C       2.774787     1.498332    -1.720909      79.54
 H       2.740296     2.391975    -2.522164      16.01
 C       3.204703     0.734354     0.538118      44.09
 H       3.108814     0.706548     1.601497      18.04
 C       3.906647    -0.382172    -0.089993       9.23
 O       4.447395    -1.196525     0.940500     217.82
 C       5.660806    -1.859830     0.815699     108.11
 H       5.538189    -2.995384     0.531113      25.22
 H       6.136804    -1.936556     1.750084      27.82
 H       6.390817    -1.513442    -0.174684      25.27
 C       4.093585    -0.616593    -1.408969      36.87
 O       4.574215    -1.792091    -1.889694     258.16
 H       5.271315    -1.546695    -2.454772      26.62
 C       3.461522     0.278371    -2.288216      12.23
 H       3.756190     0.327654    -3.267721      25.13
 C       2.544922     1.642650    -0.284274      69.57
 C       1.960608     2.972600     0.217522      95.32
 H       2.288174     3.807860    -0.702482      20.42
 O       2.243246     3.343824     1.566670     301.64
 H       3.072641     3.719257     1.710274      32.60
 C       0.442141     3.050251     0.041803      72.28
 H       0.317923     2.907734    -1.001398      20.37
 C      -0.204952     4.395924     0.606414      92.51
 O       0.484408     5.667028    -0.008244     235.53
 H       0.646387     5.526888    -0.948238      31.65
 H      -0.084797     4.575406     1.623297      26.36
 H      -1.313901     4.593793     0.256711      22.75
 C      -1.024264    -1.391355    -0.645555      27.89
 H      -0.404745    -2.320670    -0.665935      17.11
 C      -2.959048     0.030244    -0.826893      34.26
 H      -4.184342     0.149202    -0.994312      20.26
 C      -2.251029     1.060085    -0.222073       6.89
 O      -3.107364     2.312383    -0.249568     165.69
 C      -3.420421     2.881349     1.063361      98.30
 H      -4.231272     2.287488     1.298702      25.57
 H      -2.644245     2.815776     1.964031      23.52
 H      -3.593724     4.002979     0.628782      23.16
 C      -0.871878     1.056486     0.199456      13.31
 O      -0.449104     2.125178     0.823328     222.65
 C      -0.264187    -0.252316    -0.165900      35.78
 H       0.867401    -0.811197     0.343841      14.99
 C      -2.342070    -1.235065    -1.050889      26.52
 C      -3.148730    -2.510166    -1.417484      80.02
 H      -4.127065    -2.131674    -1.649040      25.36
 O      -2.594128    -3.263518    -2.612737     233.26
 H      -2.757504    -4.294775    -2.404985      14.88
 C      -3.369444    -3.516400    -0.135364      76.28
 H      -2.549300    -4.064127     0.512285      19.66
 O      -4.239486    -2.742438     0.744292     280.14
 H      -3.964320    -2.531154     1.768839      24.88
 C      -4.235703    -4.786782    -0.605622      92.25
 O      -3.450339    -5.640588    -1.607320     296.00
 H      -2.662965    -6.240489    -1.308607      27.28
 H      -5.167909    -4.752191    -1.251641      24.96
 H      -4.284704    -5.580759     0.224422      26.77
55
name = lig-etoh-frame_9
 C       2.674159     1.485338    -1.732369     102.75
 H       2.761138     2.246497    -2.483394      30.21
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 C       3.181965     0.703657     0.436963      43.61
 H       3.261450     0.790244     1.561392      21.53
 C       3.890926    -0.425416     0.012148      10.64
 O       4.462453    -1.217486     0.951126     223.63
 C       5.675517    -1.903671     0.729129     119.58
 H       5.472029    -2.920112     0.568802      27.50
 H       6.102976    -1.760663     1.848135      25.27
 H       6.317579    -1.594387     0.072758      31.44
 C       4.060978    -0.573068    -1.449064      23.96
 O       4.607731    -1.801165    -1.923280     223.58
 H       5.311992    -1.975439    -2.655643      24.37
 C       3.480383     0.360911    -2.245330      79.62
 H       3.631457     0.140243    -3.409323      18.97
 C       2.616482     1.660431    -0.395720      57.09
 C       1.918317     2.901752     0.215202     115.82
 H       2.298867     3.632680    -0.329714      21.91
 O       2.300461     3.354320     1.635581     272.40
 H       3.323590     3.656497     1.533358      26.28
 C       0.407163     3.089854     0.013944      70.37
 H       0.159011     3.083129    -1.114560      21.29
 C      -0.135525     4.472531     0.566690      99.76
 O       0.433622     5.642310     0.017116     284.83
 H       0.519827     5.507973    -0.970100      29.85
 H       0.016186     4.455324     1.722211      23.56
 H      -1.126238     4.375449     0.146972      23.65
 C      -1.075324    -1.413559    -0.615275      41.34
 H      -0.463693    -2.328887    -0.761419      17.51
 C      -2.982555     0.053995    -0.815794      43.51
 H      -3.928464    -0.146037    -1.026010      20.07
 C      -2.253631     1.140934    -0.293045      24.18
 O      -3.078667     2.263343    -0.234140     250.27
 C      -3.424789     2.879122     0.994827     123.06
 H      -4.422642     2.461310     1.554118      24.76
 H      -2.717529     2.999529     1.868423      25.04
 H      -3.534004     3.945267     1.144078      26.54
 C      -0.951729     1.092736     0.163483       1.78
 O      -0.384066     2.157424     0.792654     242.66
 C      -0.257514    -0.250912    -0.172734      22.51
 H       0.645016    -0.497871    -0.012907      18.43
 C      -2.327282    -1.217053    -1.061367      20.42
 C      -3.124480    -2.552229    -1.416319      75.32
 H      -4.264563    -2.326239    -1.588056      23.97
 O      -2.562014    -3.303835    -2.587744     251.83
 H      -2.624692    -4.271310    -2.357581      17.60
 C      -3.417333    -3.559033    -0.187848      77.80
 H      -2.574601    -3.935643     0.429831      22.44
 O      -4.267350    -2.681760     0.794952     292.15
 H      -3.751985    -2.740890     1.620731      26.70
 C      -4.230192    -4.884740    -0.597233      97.28
 O      -3.424816    -5.666392    -1.592200     304.16
 H      -2.720651    -6.209065    -0.902603      22.87
 H      -5.156789    -4.786091    -1.129087      27.39
 H      -4.440574    -5.413828     0.331720      29.24
55
name = lig-etoh-frame_10
 C       2.645193     1.439732    -1.821627      70.82
 H       2.403609     2.335626    -2.513368      27.23
 C       3.176581     0.650136     0.390874      59.04
 H       3.255848     0.983032     1.403892      22.28
 C       3.889189    -0.453374     0.048531      12.35
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 O       4.453675    -1.231259     0.970384     203.48
 C       5.696529    -1.969101     0.728435     101.97
 H       5.399834    -3.071876     0.544587      24.34
 H       6.201633    -1.775378     1.597267      27.75
 H       6.498788    -1.403668    -0.068770      25.30
 C       4.039803    -0.576413    -1.457787       7.78
 O       4.641207    -1.814764    -1.935661     179.41
 H       5.133904    -2.143774    -2.847053      24.41
 C       3.473907     0.463857    -2.251159      66.04
 H       3.377994     0.162468    -3.251579      20.31
 C       2.657354     1.694512    -0.442528      48.93
 C       1.895419     2.853734     0.230552     103.57
 H       2.447114     3.877724    -0.274168      18.80
 O       2.368149     3.347798     1.674645     267.24
 H       3.356013     3.378893     1.448384      27.83
 C       0.382822     3.149277    -0.010645      83.58
 H       0.052923     3.118726    -1.031301      22.03
 C      -0.065404     4.508593     0.525557     106.76
 O       0.408127     5.639469     0.033508     264.18
 H       0.309002     5.535170    -1.062514      25.53
 H      -0.025068     4.417201     1.573745      26.42
 H      -1.209002     4.280059     0.310704      22.75
 C      -1.013154    -1.370791    -0.577803      44.90
 H      -0.628599    -2.348620    -0.829966      18.65
 C      -2.957654    -0.002694    -0.827133      19.79
 H      -4.166460    -0.024377    -1.076783      16.38
 C      -2.322323     1.211690    -0.361323      22.22
 O      -3.054885     2.258899    -0.217991     258.62
 C      -3.461476     2.886921     1.012529     106.99
 H      -4.323859     2.606970     1.475749      27.12
 H      -2.533142     2.709478     1.733419      23.39
 H      -3.648776     4.026653     1.022910      24.91
 C      -0.984036     1.018675     0.080954       3.42
 O      -0.312103     2.185091     0.771290     192.65
 C      -0.350254    -0.225616    -0.164805      23.18
 H       1.009288    -0.148198    -0.122076      12.93
 C      -2.381775    -1.236230    -1.057848      15.87
 C      -3.133819    -2.608310    -1.408685      86.00
 H      -4.133256    -2.398196    -1.719196      24.89
 O      -2.526781    -3.318143    -2.543789     282.44
 H      -2.599723    -4.250760    -2.307209      21.24
 C      -3.498575    -3.569878    -0.225347      76.32
 H      -2.459831    -3.775056     0.264716      21.62
 O      -4.270445    -2.657515     0.821114     307.39
 H      -3.586389    -2.815475     1.491400      25.48
 C      -4.211376    -4.955965    -0.597709      84.06
 O      -3.385888    -5.704751    -1.536170     371.46
 H      -2.947409    -6.120194    -0.793159      27.57
 H      -5.226223    -4.592846    -0.998935      26.72
 H      -4.534034    -5.360763     0.411098      27.43
55
name = lig-etoh-frame_11
 C       2.630684     1.494242    -1.903157      51.28
 H       1.849267     2.110893    -2.468786      23.01
 C       3.164886     0.666704     0.391037      49.03
 H       3.164270     1.037070     1.444120      21.46
 C       3.913988    -0.484650    -0.046491      15.69
 O       4.452271    -1.261321     1.009855     199.55
 C       5.728416    -2.015565     0.711138     108.57
 H       5.535525    -3.023394     0.460114      27.36
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 H       6.455966    -1.978265     1.678385      25.69
 H       6.172388    -1.593800    -0.099871      28.91
 C       4.030128    -0.609358    -1.441729      27.50
 O       4.660946    -1.823939    -1.928860     231.36
 H       4.758779    -1.797244    -2.831152      32.20
 C       3.478149     0.466267    -2.297179      46.77
 H       3.309634     0.270931    -3.409724      17.38
 C       2.654208     1.696519    -0.440852      23.93
 C       1.944006     2.925808     0.214100     113.29
 H       2.280412     3.697266    -0.298342      24.05
 O       2.422386     3.296064     1.672700     315.95
 H       3.383820     3.257894     1.623425      30.16
 C       0.409240     3.180899    -0.025442      77.42
 H       0.139781     3.046545    -1.128684      19.94
 C      -0.091661     4.454473     0.519164     108.70
 O       0.408296     5.692752    -0.008883     294.83
 H       0.281301     5.699403    -0.895043      33.95
 H       0.077885     4.534153     1.667766      24.24
 H      -1.184713     4.513817     0.586759      24.41
 C      -0.977623    -1.326662    -0.583710      45.98
 H      -0.522322    -2.352974    -0.798746      17.62
 C      -3.013282    -0.056852    -0.871099      31.94
 H      -3.952725     0.323053    -1.005738      19.65
 C      -2.361711     1.166026    -0.405145       2.89
 O      -3.089386     2.334097    -0.228327     225.26
 C      -3.447613     2.926833     1.087170      81.59
 H      -4.483828     2.344278     1.393384      23.00
 H      -2.579248     2.423021     1.595772      22.00
 H      -3.551333     3.893502     0.556170      22.21
 C      -1.004486     0.991731    -0.001519       4.30
 O      -0.277868     2.155487     0.746499     178.22
 C      -0.351437    -0.186675    -0.140731      41.56
 H       0.582082     0.065793    -0.097214      17.52
 C      -2.408001    -1.309950    -1.006811      13.96
 C      -3.183893    -2.639197    -1.415937      73.54
 H      -4.113201    -2.207011    -2.011049      19.99
 O      -2.477573    -3.318098    -2.488170     252.56
 H      -2.603384    -4.371573    -2.298438      15.78
 C      -3.547070    -3.550655    -0.228109      84.88
 H      -2.485887    -3.714826     0.120571      20.15
 O      -4.246033    -2.684112     0.812233     296.06
 H      -3.493582    -2.646895     1.619528      21.75
 C      -4.235788    -4.929527    -0.587134      96.53
 O      -3.369767    -5.737566    -1.460459     327.29
 H      -2.781014    -6.441896    -0.705972      18.96
 H      -5.143678    -4.584836    -1.052534      25.79
 H      -4.412385    -5.551574     0.327783      26.97
55
name = lig-etoh-frame_12
 C       2.614098     1.566130    -1.899406      84.41
 H       1.743810     1.813576    -2.529932      17.91
 C       3.172337     0.724551     0.402508      26.14
 H       3.100714     0.781331     1.495942      18.35
 C       3.931718    -0.480212    -0.117508      -5.66
 O       4.464865    -1.302916     1.036333     160.12
 C       5.745893    -2.048692     0.730737     106.48
 H       5.540097    -3.130475     0.410250      25.58
 H       6.389158    -2.121837     1.523853      27.98
 H       6.125055    -1.618876    -0.351329      23.47
 C       4.024786    -0.645579    -1.455984      19.74
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 O       4.665654    -1.803376    -1.916154     172.98
 H       4.393597    -1.452022    -2.905940      22.78
 C       3.456007     0.402752    -2.382636     103.26
 H       3.531886     0.310955    -3.504149      26.06
 C       2.608690     1.678176    -0.439512      61.69
 C       2.024591     3.024478     0.204480      99.98
 H       2.406311     3.930785    -0.601777      23.52
 O       2.444743     3.216400     1.625371     288.27
 H       3.516670     3.299262     1.788698      26.50
 C       0.457041     3.143871    -0.036982      74.33
 H       0.388380     3.032065    -1.120315      22.20
 C      -0.153047     4.448255     0.586772      96.02
 O       0.423084     5.761524    -0.044802     182.22
 H       0.279818     5.811875    -1.133414      26.09
 H       0.370048     4.577564     1.530555      25.27
 H      -1.250769     4.608777     0.603342      24.32
 C      -1.003603    -1.339335    -0.633595      44.03
 H      -0.316614    -2.126458    -0.689629      20.36
 C      -3.070122    -0.055387    -0.906090      29.88
 H      -4.174848     0.341074    -1.119637      22.42
 C      -2.379408     1.076907    -0.413797       2.39
 O      -3.132450     2.396600    -0.295085     164.77
 C      -3.448988     2.896385     1.121498      99.31
 H      -4.331781     2.422044     1.317089      26.28
 H      -2.659740     2.660123     1.907380      24.33
 H      -3.449648     3.927557     0.735895      24.46
 C      -1.049757     1.076698    -0.051757      12.51
 O      -0.284479     2.072224     0.705262     183.09
 C      -0.353884    -0.158298    -0.124430       1.30
 H       0.960440    -0.002414     0.088663      12.01
 C      -2.396514    -1.392948    -0.924366      12.97
 C      -3.265818    -2.605111    -1.469775      80.46
 H      -4.041136    -2.145735    -1.989771      22.00
 O      -2.415619    -3.342831    -2.424249     281.56
 H      -2.581982    -4.248388    -2.335389      18.84
 C      -3.560399    -3.508417    -0.205251      82.76
 H      -2.551924    -3.849917     0.181008      16.85
 O      -4.193183    -2.741115     0.801723     368.90
 H      -3.720173    -2.462882     1.527353      29.19
 C      -4.250418    -4.874368    -0.559993      98.57
 O      -3.357461    -5.776692    -1.388194     372.07
 H      -2.801242    -6.310234    -0.765325      25.48
 H      -5.180972    -4.793496    -1.256024      23.84
 H      -4.417348    -5.559418     0.255121      25.57
55
name = lig-etoh-frame_13
 C       2.651883     1.532116    -1.863117      77.56
 H       1.857690     1.778881    -2.694186      17.21
 C       3.222288     0.733083     0.399671      36.60
 H       3.071281     0.607524     1.472442      18.63
 C       3.917868    -0.418074    -0.062512      -8.51
 O       4.482856    -1.333709     1.021655     170.74
 C       5.719037    -2.088868     0.680528     105.80
 H       5.386529    -3.113086     0.517463      25.73
 H       6.452909    -2.027555     1.605293      25.83
 H       6.274461    -1.667995    -0.179318      26.56
 C       4.011048    -0.642350    -1.500367       3.32
 O       4.654175    -1.749038    -1.955260     176.47
 H       4.335007    -1.779778    -2.966427      20.91
 C       3.400883     0.352816    -2.426942      96.97
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 H       3.721386     0.235935    -3.479133      28.43
 C       2.545868     1.696265    -0.443658      78.61
 C       2.121190     3.126075     0.167846     112.48
 H       2.470997     3.862439    -0.396084      27.67
 O       2.462807     3.138112     1.552405     336.20
 H       3.365757     3.426392     1.574299      30.65
 C       0.503596     3.103365    -0.014811      65.54
 H       0.446939     3.056133    -1.126107      22.38
 C      -0.155734     4.503562     0.622807      82.31
 O       0.428459     5.819108    -0.094489     190.18
 H       0.325652     5.671872    -1.089768      28.37
 H       0.420863     4.532860     1.554441      24.53
 H      -1.307295     4.473768     0.585410      23.04
 C      -1.022496    -1.338179    -0.662094      27.95
 H      -0.213637    -2.160768    -0.676115      18.42
 C      -3.122959    -0.053111    -0.920809      36.34
 H      -4.140172    -0.143917    -1.256688      25.08
 C      -2.444920     1.056710    -0.407932       3.75
 O      -3.148782     2.412920    -0.365708     153.10
 C      -3.413417     2.858255     1.101288     103.03
 H      -4.508263     2.502520     1.448499      23.84
 H      -2.826889     3.000507     2.103218      23.03
 H      -3.549545     4.030600     1.314567      24.30
 C      -1.029293     1.142742    -0.063368      10.43
 O      -0.307540     1.989093     0.646402     198.48
 C      -0.328988    -0.120904    -0.135426       7.39
 H       0.576757    -0.429652     0.249972      17.47
 C      -2.418576    -1.409138    -0.874060      11.47
 C      -3.269074    -2.563572    -1.493707      61.43
 H      -4.286515    -2.147732    -1.982602      21.02
 O      -2.354580    -3.350467    -2.363860     202.28
 H      -2.647361    -4.363115    -2.282239      12.71
 C      -3.544947    -3.480450    -0.189295      75.29
 H      -2.571362    -3.978116     0.199230      15.21
 O      -4.184419    -2.798838     0.785838     333.57
 H      -3.603926    -2.397202     1.540267      23.50
 C      -4.272400    -4.842224    -0.566519      93.14
 O      -3.382490    -5.764701    -1.380729     313.01
 H      -2.720779    -6.160550    -0.484350      18.38
 H      -5.105845    -4.939037    -1.238636      24.23
 H      -4.651680    -5.337530     0.435354      25.55
55
name = lig-etoh-frame_14
 C       2.699088     1.416731    -1.862940      58.65
 H       2.209730     2.088604    -2.575663      18.37
 C       3.265452     0.724189     0.396968      56.77
 H       3.064795     0.758377     1.494897      18.70
 C       3.918044    -0.373460    -0.006076       5.22
 O       4.491377    -1.331179     0.966347     192.32
 C       5.685574    -2.120886     0.666373     111.31
 H       5.331889    -3.169751     0.579267      25.56
 H       6.281750    -1.916093     1.530816      27.50
 H       6.397503    -1.715158    -0.171986      25.85
 C       3.971043    -0.580201    -1.525378      12.75
 O       4.640632    -1.712902    -2.029839     224.55
 H       4.480752    -2.157237    -2.824770      26.07
 C       3.351810     0.304901    -2.388149      29.05
 H       3.729413     0.215396    -3.477507      25.98
 C       2.530919     1.725225    -0.459705      68.42
 C       2.134879     3.104263     0.147770      98.44
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 H       2.643207     4.142914    -0.385332      22.59
 O       2.479128     3.082098     1.476637     285.72
 H       3.410234     3.538862     1.454430      27.21
 C       0.532582     3.124767     0.012460      67.78
 H       0.268575     3.079324    -1.077783      20.54
 C      -0.092929     4.559315     0.602024      92.80
 O       0.415169     5.833227    -0.128534     225.29
 H       0.365551     5.559786    -1.050471      30.46
 H       0.157197     4.585917     1.733190      24.48
 H      -1.137249     4.413053     0.618615      25.32
 C      -1.011766    -1.316509    -0.651100      39.19
 H      -0.537608    -2.259917    -0.755911      20.09
 C      -3.129763    -0.114368    -0.904441      36.50
 H      -4.146108    -0.351482    -1.310587      24.56
 C      -2.520355     1.124578    -0.400748      -6.29
 O      -3.147560     2.412049    -0.385390     185.08
 C      -3.438601     2.877653     1.106547     103.70
 H      -4.374567     2.478812     1.439104      25.82
 H      -2.674467     2.651902     1.888064      25.19
 H      -3.716412     3.895675     1.235281      26.47
 C      -1.003723     1.078634    -0.090040      14.69
 O      -0.297002     1.986342     0.611125     181.68
 C      -0.404665    -0.144710    -0.192568      29.39
 H       0.609491    -0.555949     0.459457      16.21
 C      -2.459173    -1.341285    -0.892004      18.49
 C      -3.217060    -2.544863    -1.467083      79.72
 H      -4.157234    -2.364576    -1.875701      23.89
 O      -2.315356    -3.357256    -2.308725     236.03
 H      -2.678702    -4.284610    -2.184777      16.85
 C      -3.513343    -3.510042    -0.229633      82.00
 H      -2.515388    -3.852989     0.109631      18.30
 O      -4.215051    -2.828898     0.813486     328.47
 H      -3.385849    -2.524162     1.396229      21.95
 C      -4.307753    -4.834549    -0.573144      83.15
 O      -3.408940    -5.724785    -1.349836     362.07
 H      -2.789382    -6.218140    -0.657065      25.68
 H      -5.250706    -4.706490    -1.228983      26.06
 H      -4.677890    -5.069731     0.394028      26.73
55
name = lig-etoh-frame_15
 C       2.695523     1.362566    -1.853972      76.67
 H       2.729784     2.420562    -2.393898      18.80
 C       3.244676     0.775386     0.428660      53.84
 H       3.186275     1.035058     1.466190      20.01
 C       3.962000    -0.402269    -0.035054      11.40
 O       4.478236    -1.292576     0.883530     209.15
 C       5.647115    -2.128031     0.663655     109.06
 H       5.447925    -3.229674     0.570663      26.02
 H       6.215982    -1.982714     1.644637      26.35
 H       6.310486    -1.900576    -0.279279      25.40
 C       3.939775    -0.568399    -1.506376      15.73
 O       4.649788    -1.669949    -2.070049     201.91
 H       4.376843    -2.486049    -2.789202      22.87
 C       3.328163     0.260055    -2.356218      14.63
 H       3.459606     0.236875    -3.380385      22.14
 C       2.607642     1.697529    -0.502746      47.63
 C       2.092509     3.038827     0.080505     116.05
 H       2.445798     3.900272    -0.310859      21.41
 O       2.517746     3.056312     1.438011     294.52
 H       3.453628     3.475811     1.604526      28.03
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 C       0.526791     3.204571     0.018163      65.55
 H       0.183989     3.169550    -1.005094      19.82
 C       0.005946     4.592564     0.585847      99.43
 O       0.386599     5.805101    -0.134277     207.55
 H       0.442171     5.508791    -1.212812      24.71
 H       0.033538     4.783868     1.636203      24.75
 H      -1.180293     4.483520     0.454257      22.09
 C      -1.079323    -1.328289    -0.644668      53.08
 H      -0.715344    -2.376454    -0.768985      18.22
 C      -3.143677    -0.134328    -0.861201      34.70
 H      -4.218734    -0.070157    -1.221439      20.61
 C      -2.541109     1.192097    -0.406874      -5.12
 O      -3.150972     2.408103    -0.363720     214.18
 C      -3.464925     2.876404     1.109932      63.24
 H      -4.381036     2.168528     1.406887      23.59
 H      -2.523366     2.232134     1.374189      21.10
 H      -3.688965     4.004109     0.807419      21.77
 C      -1.062828     0.995651    -0.133477      -1.90
 O      -0.255427     2.044074     0.608765     147.37
 C      -0.433773    -0.255674    -0.224608      38.39
 H       0.497513    -0.117141     0.362349      17.18
 C      -2.443993    -1.263452    -0.959825      36.25
 C      -3.120086    -2.570942    -1.387546      77.16
 H      -4.136063    -2.390112    -1.995548      22.11
 O      -2.288619    -3.353783    -2.261400     252.18
 H      -2.591253    -4.262223    -2.153717      20.42
 C      -3.496591    -3.551038    -0.290479      80.75
 H      -2.402444    -3.745479     0.089170      18.35
 O      -4.226936    -2.851714     0.855079     332.81
 H      -3.544622    -2.610098     1.399056      27.18
 C      -4.334833    -4.799172    -0.606697      76.00
 O      -3.461183    -5.670843    -1.320232     359.34
 H      -2.850981    -6.427321    -0.791513      23.25
 H      -5.194913    -4.371288    -1.145528      27.14
 H      -4.638889    -5.179171     0.466864      25.88
55
name = lig-etoh-frame_16
 C       2.683688     1.437290    -1.851396      72.59
 H       2.933151     2.256090    -2.428644      26.54
 C       3.225253     0.810720     0.443964      44.62
 H       3.382543     1.192189     1.482695      20.56
 C       3.977723    -0.402777    -0.110411       9.78
 O       4.461672    -1.254758     0.803884     212.59
 C       5.626698    -2.137894     0.670579     115.13
 H       5.365880    -3.195063     0.578375      26.44
 H       6.211557    -2.095444     1.618575      26.47
 H       6.157500    -1.920187    -0.270520      26.08
 C       3.933583    -0.662066    -1.456333      21.06
 O       4.690158    -1.651686    -2.100674     267.75
 H       4.007774    -2.258881    -2.436131      28.76
 C       3.292606     0.252856    -2.353327      38.36
 H       3.222489     0.126673    -3.538440      19.32
 C       2.715328     1.634719    -0.508598      40.16
 C       2.030155     2.926281     0.030607     113.33
 H       2.437332     3.929357    -0.644328      21.04
 O       2.552760     3.049482     1.446802     291.88
 H       3.438721     3.355436     1.520242      31.28
 C       0.503537     3.270291     0.010914      63.79
 H       0.252627     3.353252    -1.110901      19.68
 C       0.030832     4.608894     0.554970     109.07
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 O       0.377039     5.759088    -0.164597     284.23
 H       0.454008     5.664102    -1.062778      33.48
 H       0.211471     4.957564     1.652016      23.62
 H      -0.976209     4.550170     0.306426      24.38
 C      -1.168198    -1.427618    -0.654945      43.86
 H      -0.649334    -2.393008    -0.677964      17.43
 C      -3.199485    -0.014549    -0.805640      39.09
 H      -4.213730     0.175293    -1.033176      17.52
 C      -2.491974     1.180159    -0.433521       8.94
 O      -3.175185     2.401166    -0.357115     248.58
 C      -3.481179     2.810180     1.045585     105.73
 H      -4.307698     2.181697     1.408917      25.94
 H      -2.546136     2.547233     1.467902      26.73
 H      -3.488062     3.809930     0.871022      26.32
 C      -1.159777     0.983241    -0.160569      -7.25
 O      -0.223019     2.098195     0.612832     102.04
 C      -0.426723    -0.280659    -0.213817      17.90
 H       0.678298    -0.028560     0.187669      14.88
 C      -2.428422    -1.250248    -1.045684      32.01
 C      -3.086327    -2.599024    -1.352835     105.89
 H      -3.868430    -2.261789    -1.955058      24.74
 O      -2.245017    -3.345718    -2.231314     240.86
 H      -2.454301    -4.383376    -2.156565      17.58
 C      -3.465259    -3.545910    -0.257278     101.26
 H      -2.538480    -3.913571     0.148939      23.05
 O      -4.235938    -2.885490     0.868143     306.24
 H      -3.606647    -2.590315     1.696678      22.83
 C      -4.326746    -4.741124    -0.588402      98.60
 O      -3.523747    -5.646085    -1.338761     382.27
 H      -3.111692    -6.174593    -0.694337      30.86
 H      -5.187367    -4.355877    -1.207573      26.83
 H      -4.610406    -5.302958     0.236999      27.92
55
name = lig-etoh-frame_17
 C       2.721764     1.480805    -1.902021      41.37
 H       2.697940     2.315112    -2.769457      22.80
 C       3.278715     0.758956     0.437878      32.80
 H       3.486345     1.079952     1.432313      21.97
 C       3.948182    -0.350504    -0.146254      20.94
 O       4.461464    -1.239119     0.770776     203.00
 C       5.598382    -2.152184     0.674950     104.26
 H       5.105879    -3.172690     0.579885      24.07
 H       6.248820    -2.042407     1.539677      26.34
 H       6.225350    -1.814050    -0.335639      23.77
 C       3.910547    -0.727586    -1.476378      22.31
 O       4.723489    -1.658378    -2.118175     274.75
 H       3.878966    -2.159134    -2.234958      25.76
 C       3.239917     0.259281    -2.365450      26.23
 H       3.221387    -0.017795    -3.343385      19.58
 C       2.752703     1.638382    -0.464116      59.70
 C       2.028705     2.882207     0.004273     119.89
 H       2.390333     3.524345    -0.702499      25.37
 O       2.552542     3.060377     1.457112     247.78
 H       3.580558     3.343519     1.250972      25.60
 C       0.496713     3.262984    -0.034842      69.90
 H       0.371219     3.409492    -1.081329      20.04
 C       0.023342     4.627350     0.547130      96.03
 O       0.405642     5.759276    -0.194250     252.95
 H       0.423284     5.664685    -1.278891      25.36
 H       0.378803     4.788562     1.519633      25.03
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 H      -1.181597     4.471665     0.456819      21.33
 C      -1.143184    -1.482973    -0.630926      14.43
 H      -0.627402    -2.429484    -0.635231      17.11
 C      -3.216371     0.095210    -0.776574      36.79
 H      -4.378212     0.238613    -0.881138      15.60
 C      -2.472160     1.150255    -0.467198      18.47
 O      -3.200708     2.380667    -0.370260     228.70
 C      -3.447302     2.719591     0.963635     113.17
 H      -4.403362     2.298516     1.476158      24.48
 H      -2.610216     2.914821     1.919344      22.01
 H      -3.586459     3.952341     1.140131      23.39
 C      -1.133283     1.001355    -0.141469       1.79
 O      -0.226757     2.134294     0.604089     113.38
 C      -0.446339    -0.236781    -0.184744      25.84
 H       0.737393    -0.343736    -0.201216      16.96
 C      -2.504085    -1.246617    -1.095138       6.13
 C      -3.089552    -2.601013    -1.367177      86.18
 H      -4.049956    -2.253796    -1.979770      23.03
 O      -2.176792    -3.360272    -2.223528     237.42
 H      -2.383066    -4.276657    -2.108186      18.66
 C      -3.449958    -3.505677    -0.119460      83.67
 H      -2.556097    -4.170681     0.313955      18.28
 O      -4.231612    -2.911014     0.881444     328.24
 H      -3.736464    -2.711932     1.733790      25.60
 C      -4.326816    -4.668624    -0.592913      92.44
 O      -3.588263    -5.635424    -1.403436     313.01
 H      -3.085957    -6.074532    -0.502670      21.92
 H      -5.220275    -4.508965    -1.251144      25.04
 H      -4.781240    -5.317750     0.283577      25.83
55
name = lig-etoh-frame_18
 C       2.790905     1.503901    -1.973482      40.71
 H       2.208722     2.126692    -2.611815      14.06
 C       3.360858     0.693424     0.404628      41.76
 H       3.460252     0.821405     1.500101      19.59
 C       3.939275    -0.353377    -0.152367      13.14
 O       4.472049    -1.228513     0.789527     215.10
 C       5.561710    -2.144979     0.629979     122.08
 H       5.164294    -3.125373     0.587734      26.55
 H       6.250418    -1.971566     1.544557      26.22
 H       6.202684    -1.957594    -0.164368      27.45
 C       3.859105    -0.667701    -1.543185      29.41
 O       4.730147    -1.687656    -2.129530     177.94
 H       4.069474    -2.602820    -2.333610      22.74
 C       3.207957     0.242089    -2.349321      54.95
 H       3.310547    -0.062600    -3.475544      27.06
 C       2.713842     1.682604    -0.464119      40.56
 C       2.052648     2.865279     0.051422     106.22
 H       2.586506     3.688671    -0.761972      23.33
 O       2.554072     3.099167     1.428932     285.11
 H       3.474834     3.358626     1.281976      30.31
 C       0.510672     3.196088    -0.091056      67.15
 H       0.318478     3.240474    -1.233654      19.60
 C      -0.026626     4.611379     0.528649      97.80
 O       0.456680     5.790923    -0.246970     259.84
 H       0.303063     5.525216    -1.227132      28.31
 H       0.501730     4.597456     1.571910      25.04
 H      -1.024949     4.498999     0.796246      26.46
 C      -1.123230    -1.410210    -0.598398      26.17
 H      -0.663427    -2.448279    -0.665895      17.45
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 C      -3.243871     0.059265    -0.810536      40.32
 H      -4.259963     0.168005    -0.796919      17.32
 C      -2.459979     1.185827    -0.472604      -2.36
 O      -3.201601     2.355921    -0.378729     247.63
 C      -3.418016     2.740187     0.989918     130.93
 H      -4.396895     2.289936     1.370035      25.52
 H      -2.793668     2.689387     1.761981      28.99
 H      -3.872559     3.672202     0.973255      27.29
 C      -0.989455     1.057073    -0.081574       9.74
 O      -0.273602     2.143690     0.572934     193.23
 C      -0.474641    -0.240991    -0.196987      39.25
 H       0.612213    -0.437428    -0.260602      18.54
 C      -2.556682    -1.233666    -1.058783       2.96
 C      -3.145110    -2.581480    -1.413989      70.39
 H      -4.127012    -2.660084    -1.833210      24.72
 O      -2.109821    -3.363910    -2.218079     198.09
 H      -2.434141    -4.326663    -2.062117      15.22
 C      -3.444356    -3.506059     0.013190      87.52
 H      -2.588777    -3.956731     0.389631      24.68
 O      -4.238526    -2.913076     0.918279     366.10
 H      -3.713179    -2.778726     1.693964      28.23
 C      -4.376221    -4.647572    -0.611780      88.91
 O      -3.631269    -5.634557    -1.437843     370.03
 H      -2.942677    -6.157072    -0.997205      31.14
 H      -5.230274    -4.348729    -1.226647      27.50
 H      -4.790509    -5.020186     0.273545      28.07
55
name = lig-etoh-frame_19
 C       2.816164     1.516989    -1.952047      41.08
 H       1.857145     1.967494    -2.429990      17.95
 C       3.386019     0.735205     0.365528      27.42
 H       3.311509     0.603990     1.463363      20.11
 C       3.976886    -0.457838    -0.190274       5.05
 O       4.484202    -1.218244     0.828138     206.97
 C       5.537906    -2.122275     0.615719     118.02
 H       5.301314    -3.266656     0.629077      25.17
 H       6.092398    -2.024632     1.509559      27.84
 H       6.322768    -2.053965    -0.378147      23.15
 C       3.843826    -0.620107    -1.590179      22.30
 O       4.696158    -1.742331    -2.139496     260.55
 H       4.587119    -2.580577    -2.367988      29.50
 C       3.202542     0.218606    -2.415665      70.67
 H       3.311661     0.116764    -3.457248      28.33
 C       2.688782     1.664889    -0.524763      36.93
 C       2.105067     2.943003     0.093952     122.03
 H       2.482730     3.780105    -0.341782      24.53
 O       2.534177     3.148394     1.392740     287.62
 H       3.504718     3.470000     1.463596      28.70
 C       0.515457     3.122935    -0.168134      64.61
 H       0.269313     2.954335    -1.184738      23.21
 C       0.006186     4.564491     0.526200      86.04
 O       0.489324     5.796682    -0.281684     250.81
 H       0.321425     5.577292    -1.188539      30.35
 H       0.573288     4.597338     1.413551      26.18
 H      -1.129065     4.629097     0.930296      23.70
 C      -1.199703    -1.301066    -0.601019      56.75
 H      -0.712177    -2.214995    -0.705841      19.47
 C      -3.205873    -0.040229    -0.863945      28.64
 H      -4.380925     0.086429    -0.860659      20.57
 C      -2.401326     1.210493    -0.447153     -20.83
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 O      -3.177074     2.340410    -0.378062     199.91
 C      -3.480131     2.776201     1.017013      71.75
 H      -4.344688     1.986264     1.293225      22.86
 H      -2.449558     2.362317     1.715603      20.40
 H      -4.008907     3.803151     0.698153      21.82
 C      -0.906452     1.131961    -0.040119      13.84
 O      -0.336784     2.135341     0.537625     215.20
 C      -0.461659    -0.249596    -0.219780      30.17
 H       0.772221    -0.376097     0.027742      16.77
 C      -2.567355    -1.230856    -0.974464      30.04
 C      -3.180442    -2.583155    -1.416946      44.04
 H      -4.169022    -2.862645    -1.896360      20.47
 O      -2.073461    -3.363530    -2.195417     180.41
 H      -2.484895    -4.312293    -2.150925      16.06
 C      -3.459342    -3.534706     0.018099      70.52
 H      -2.358102    -3.731919     0.504887      19.13
 O      -4.268949    -2.883083     0.994831     304.26
 H      -3.604966    -2.663382     1.848769      21.23
 C      -4.391252    -4.658473    -0.612987      65.39
 O      -3.684641    -5.620742    -1.492855     346.33
 H      -2.944765    -6.208527    -1.154887      27.25
 H      -5.142572    -4.027582    -1.236660      25.51
 H      -4.869879    -5.053567     0.371320      25.55
55
name = lig-etoh-frame_20
 C       2.752849     1.496155    -1.895215      51.91
 H       1.961671     1.943302    -2.456935      19.17
 C       3.380973     0.768024     0.290867      41.11
 H       3.158298     0.728118     1.349931      20.63
 C       3.978473    -0.503912    -0.219834       8.44
 O       4.494171    -1.219320     0.851935     212.97
 C       5.575344    -2.154399     0.593192     123.22
 H       5.219691    -3.149939     0.616398      27.09
 H       6.177142    -2.051828     1.597343      25.88
 H       6.041871    -1.924470    -0.234324      27.78
 C       3.898948    -0.702035    -1.617814      13.07
 O       4.673757    -1.743127    -2.144312     233.24
 H       4.674556    -2.787905    -2.399968      22.05
 C       3.206637     0.264470    -2.515730      56.60
 H       3.233804     0.162085    -3.636076      27.18
 C       2.713659     1.636031    -0.555864      59.66
 C       2.133109     3.022789     0.096444     103.04
 H       2.464210     4.098465    -0.447804      21.75
 O       2.506806     3.194226     1.415588     273.42
 H       3.474626     3.599318     1.565610      26.97
 C       0.508773     3.079441    -0.192425      65.82
 H       0.301145     2.844033    -1.304585      20.93
 C       0.069271     4.521526     0.491950      87.73
 O       0.506622     5.769078    -0.278313     201.21
 H       0.379525     5.707741    -1.392047      24.59
 H       0.744084     4.659857     1.406718      24.25
 H      -0.937374     4.654570     0.624098      26.03
 C      -1.281935    -1.223807    -0.623738      43.76
 H      -0.676250    -2.177551    -0.760886      17.95
 C      -3.161273    -0.042640    -0.882804      33.01
 H      -4.188794     0.017674    -1.076083      26.25
 C      -2.335717     1.165399    -0.420668       3.10
 O      -3.136483     2.339245    -0.380080     224.27
 C      -3.557401     2.761041     1.025584     107.62
 H      -4.149715     1.885746     1.355308      25.35
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 H      -2.660024     2.682054     1.412984      28.39
 H      -3.773719     3.770436     0.944613      26.52
 C      -0.971978     1.108064    -0.073019      13.11
 O      -0.362569     2.163441     0.541297     224.25
 C      -0.367297    -0.175342    -0.195703      32.13
 H       0.581875    -0.353251     0.202351      18.18
 C      -2.584634    -1.285313    -0.915132      36.21
 C      -3.171225    -2.626391    -1.363052      65.13
 H      -4.015555    -2.500417    -2.097151      19.59
 O      -2.077781    -3.357073    -2.154374     224.54
 H      -2.431504    -4.211606    -2.297230      20.50
 C      -3.451214    -3.542593    -0.028902      98.31
 H      -2.534677    -3.693669     0.345123      23.67
 O      -4.285714    -2.842350     1.092836     331.90
 H      -3.716701    -2.546636     1.767649      28.25
 C      -4.367007    -4.676087    -0.561948     100.89
 O      -3.756078    -5.591864    -1.571203     329.51
 H      -3.149782    -6.124538    -0.827398      24.14
 H      -5.005707    -4.097405    -1.146091      27.61
 H      -4.937138    -5.293187     0.117173      26.79
55
name = lig-etoh-frame_21
 C       2.653069     1.410203    -1.926400      46.60
 H       2.187052     2.198912    -2.654952      25.10
 C       3.374467     0.728446     0.215862      34.83
 H       3.187235     1.025557     1.292610      19.88
 C       3.936963    -0.463270    -0.226834      13.87
 O       4.498591    -1.227927     0.860911     174.07
 C       5.614248    -2.187284     0.642908     100.72
 H       5.112018    -3.211410     0.495680      24.56
 H       6.329588    -2.094703     1.399067      27.62
 H       6.076261    -1.702262    -0.443729      22.60
 C       3.942467    -0.800398    -1.666598      27.47
 O       4.693586    -1.749596    -2.174328     226.09
 H       4.251809    -2.729173    -2.246656      26.09
 C       3.249010     0.315505    -2.563214      64.41
 H       3.114663     0.119677    -3.656837      19.16
 C       2.754197     1.688734    -0.516777      32.05
 C       2.144494     3.087513     0.026569      86.98
 H       2.361512     3.850915    -0.657492      23.72
 O       2.480074     3.242430     1.486768     319.36
 H       3.337404     3.611638     1.459431      29.27
 C       0.511803     3.079603    -0.179703      80.16
 H       0.426903     3.037291    -1.238819      21.57
 C       0.185329     4.499390     0.397501      93.71
 O       0.527118     5.732283    -0.287476     281.16
 H       0.448378     5.693489    -1.196642      32.17
 H       0.636599     4.599687     1.391504      24.53
 H      -1.002289     4.522625     0.417630      22.70
 C      -1.199354    -1.199894    -0.618487      24.85
 H      -0.729133    -2.146711    -0.739778      20.80
 C      -3.105385     0.024756    -0.872782      39.48
 H      -4.174218     0.189507    -1.285965      25.73
 C      -2.371081     1.094556    -0.421803      24.45
 O      -3.091339     2.345535    -0.391103     188.02
 C      -3.595186     2.705906     0.986648      83.45
 H      -4.295562     1.979624     1.548928      24.21
 H      -2.457718     3.014033     1.676869      20.22
 H      -3.894181     3.861033     1.216554      23.30
 C      -1.047853     1.047886    -0.114248      20.69
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 O      -0.370379     2.205313     0.567851     184.15
 C      -0.353688    -0.096659    -0.186428      35.99
 H       0.710799    -0.469827     0.439658      15.84
 C      -2.612947    -1.338066    -0.887033      19.54
 C      -3.135053    -2.668160    -1.301471      92.25
 H      -3.842354    -2.185509    -2.038973      18.66
 O      -2.101800    -3.333839    -2.095817     207.76
 H      -2.477945    -4.259731    -2.436046      16.80
 C      -3.496103    -3.510547    -0.074309      85.59
 H      -2.403780    -3.915212     0.330615      17.07
 O      -4.299710    -2.820098     1.137990     264.17
 H      -3.573940    -2.474950     1.838444      22.76
 C      -4.349254    -4.697663    -0.530842      98.31
 O      -3.804944    -5.568185    -1.604983     324.41
 H      -3.377453    -6.076967    -0.986003      30.43
 H      -5.253224    -4.182007    -1.121093      24.39
 H      -4.910771    -5.461321     0.066522      24.99
55
name = lig-etoh-frame_22
 C       2.549260     1.358056    -2.002100      87.80
 H       2.564418     2.252574    -2.626890      27.41
 C       3.343470     0.716312     0.217065      38.84
 H       3.540988     1.027075     1.230207      22.03
 C       3.919967    -0.456328    -0.258411      -2.10
 O       4.497029    -1.235009     0.869469     172.58
 C       5.628878    -2.175855     0.613664     121.12
 H       5.343010    -3.186718     0.413261      27.42
 H       6.493637    -2.155323     1.395898      26.55
 H       6.127637    -1.963265    -0.196542      29.21
 C       3.914965    -0.768759    -1.686018      15.34
 O       4.724464    -1.808463    -2.230480     284.42
 H       4.061462    -2.438757    -2.150790      30.29
 C       3.313560     0.293155    -2.542644      43.86
 H       3.138259     0.114920    -3.576962      20.13
 C       2.772483     1.781810    -0.538306       6.29
 C       2.122246     3.033092    -0.019804      69.92
 H       2.496896     3.879273    -0.841651      20.28
 O       2.442844     3.295992     1.523831     257.87
 H       3.459551     3.672827     1.457849      24.02
 C       0.561476     3.120730    -0.147079      73.24
 H       0.390282     3.172534    -1.283258      19.73
 C       0.220627     4.492885     0.299932     110.82
 O       0.574725     5.702491    -0.280202     276.01
 H       0.452528     5.577853    -1.345579      26.48
 H       0.461065     4.511185     1.386564      24.84
 H      -0.816746     4.342604     0.405303      25.14
 C      -1.081922    -1.235864    -0.595441      36.69
 H      -0.575884    -2.227102    -0.627321      20.32
 C      -3.124729     0.020002    -0.885688      52.17
 H      -4.039468     0.448867    -1.329171      24.73
 C      -2.470445     1.095511    -0.426375      14.67
 O      -3.063317     2.361026    -0.381329     230.84
 C      -3.533950     2.701606     0.994887     117.79
 H      -4.324541     2.108447     1.564365      25.54
 H      -2.906715     2.854426     1.691648      29.65
 H      -4.235206     3.544368     0.940385      26.62
 C      -1.044812     1.078533    -0.096538       0.66
 O      -0.385183     2.225546     0.580414     166.75
 C      -0.350443    -0.128406    -0.166502      39.33
 H       0.503477    -0.238853     0.245736      20.14
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 C      -2.531092    -1.286959    -0.841445      22.71
 C      -3.101660    -2.652106    -1.264772      88.72
 H      -4.024905    -2.362136    -1.866026      20.26
 O      -2.129389    -3.326484    -2.041523     254.51
 H      -2.582908    -4.137394    -2.370331      19.03
 C      -3.537286    -3.504065    -0.051286     101.28
 H      -2.696416    -3.962982     0.272533      22.18
 O      -4.283423    -2.811686     1.135049     304.77
 H      -3.487643    -2.640411     1.782681      23.21
 C      -4.427203    -4.709363    -0.554542     101.25
 O      -3.840151    -5.533631    -1.626762     280.82
 H      -3.242793    -6.392225    -1.255272      25.29
 H      -5.342515    -4.352922    -0.883896      27.99
 H      -4.628103    -5.363060     0.367246      26.42
55
name = lig-etoh-frame_23
 C       2.526261     1.368279    -2.024589      88.05
 H       2.560141     2.204955    -2.752556      26.67
 C       3.309587     0.769977     0.251385      38.18
 H       3.861606     0.852275     1.246742      21.12
 C       3.931427    -0.489466    -0.291967     -16.25
 O       4.500793    -1.243119     0.852572     143.13
 C       5.649748    -2.153737     0.595192     105.68
 H       5.379249    -3.247505     0.510459      25.47
 H       6.247346    -2.130389     1.490272      27.04
 H       6.359223    -1.953002    -0.419067      23.58
 C       3.891113    -0.666466    -1.679214      21.54
 O       4.740648    -1.858026    -2.285125     155.94
 H       3.874612    -2.582950    -2.182156      22.72
 C       3.348397     0.226954    -2.482771      41.12
 H       3.376792     0.075787    -3.635313      19.55
 C       2.767120     1.777294    -0.628949      16.12
 C       2.109232     2.964456    -0.035461     107.54
 H       2.538748     3.823040    -0.498116      20.40
 O       2.429222     3.355374     1.498505     291.49
 H       3.356843     3.613259     1.622253      28.70
 C       0.634830     3.155751    -0.175020      68.60
 H       0.294720     3.034909    -1.190461      21.08
 C       0.181327     4.487890     0.296714      97.16
 O       0.644297     5.682856    -0.308363     278.75
 H       0.516371     5.609186    -1.344691      26.58
 H       0.429698     4.556909     1.391608      24.26
 H      -0.990961     4.386305     0.296407      22.87
 C      -1.004972    -1.327703    -0.562895      56.45
 H      -0.410926    -2.247801    -0.472188      19.49
 C      -3.179872    -0.029925    -0.912765      42.26
 H      -4.153427     0.291879    -1.328233      23.43
 C      -2.471038     1.171265    -0.398128      -9.82
 O      -3.060129     2.384414    -0.345692     213.77
 C      -3.552247     2.706792     0.974845      75.42
 H      -4.227126     1.814262     1.312761      23.78
 H      -2.672349     2.810996     1.990762      20.33
 H      -4.333017     3.461362     0.516019      21.81
 C      -1.033595     1.147185    -0.048836       1.16
 O      -0.397679     2.229086     0.573118     161.77
 C      -0.394462    -0.158525    -0.154883       5.81
 H       0.894207    -0.002143     0.138436      13.77
 C      -2.379823    -1.207183    -0.815114      26.54
 C      -3.111320    -2.569343    -1.217190      71.37
 H      -4.144682    -2.638344    -1.731638      20.06
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 O      -2.152466    -3.331270    -2.001368     244.85
 H      -2.672547    -4.111452    -2.235432      20.33
 C      -3.614048    -3.513549    -0.010921      71.14
 H      -2.638419    -4.075658     0.459617      16.73
 O      -4.238163    -2.825160     1.085952     347.80
 H      -3.577755    -2.769113     1.783367      25.47
 C      -4.494103    -4.741600    -0.530696      85.24
 O      -3.866219    -5.506451    -1.647299     310.87
 H      -3.287301    -6.301128    -1.465374      30.02
 H      -5.615345    -4.464333    -0.808464      26.69
 H      -4.371284    -5.179581     0.465205      27.00
55
name = lig-etoh-frame_24
 C       2.603564     1.392315    -2.032557      79.92
 H       2.194264     2.042589    -2.878384      22.55
 C       3.340985     0.784767     0.255159      58.82
 H       3.742881     0.934173     1.243374      22.61
 C       3.924895    -0.476777    -0.250970       5.63
 O       4.507559    -1.247878     0.782641     194.50
 C       5.682988    -2.143368     0.561012     109.87
 H       5.238694    -3.135677     0.601195      25.61
 H       6.084105    -1.977344     1.619400      25.49
 H       6.240356    -1.795486    -0.240297      27.44
 C       3.955590    -0.674299    -1.641206      18.57
 O       4.689782    -1.878611    -2.314015     236.60
 H       4.199167    -2.703608    -2.377025      26.53
 C       3.301089     0.232603    -2.493860      33.86
 H       3.638476     0.049632    -3.461404      22.71
 C       2.740345     1.682995    -0.695069      47.96
 C       2.131789     2.937032     0.017974     132.95
 H       2.540272     3.954105    -0.406512      16.95
 O       2.404382     3.385714     1.444544     303.89
 H       3.389944     3.587763     1.574829      28.24
 C       0.655305     3.155067    -0.229456      50.10
 H       0.351917     2.862293    -1.266296      18.82
 C       0.075559     4.505082     0.351566     100.99
 O       0.726312     5.670715    -0.349671     279.15
 H       0.640921     5.684033    -1.313191      28.50
 H       0.415819     4.644977     1.352547      24.73
 H      -0.961640     4.599199     0.099726      23.69
 C      -0.934832    -1.391319    -0.501405      39.44
 H      -0.415040    -2.328300    -0.423585      19.06
 C      -3.157796    -0.014702    -0.895497      29.55
 H      -4.269098    -0.281156    -1.237756      22.71
 C      -2.409338     1.211309    -0.383328       0.57
 O      -3.056019     2.422121    -0.318828     245.20
 C      -3.612279     2.693255     0.985551      97.20
 H      -3.978954     1.651954     1.048896      23.17
 H      -2.901482     2.957794     1.563674      28.70
 H      -4.210703     3.566684     0.672933      24.00
 C      -1.043409     1.160113    -0.008818       5.15
 O      -0.393510     2.230639     0.563720     182.68
 C      -0.356227    -0.110544    -0.118913      24.45
 H       0.578129    -0.064603    -0.099149      19.56
 C      -2.316646    -1.197917    -0.846149      10.19
 C      -3.131044    -2.493193    -1.143630      71.68
 H      -4.061961    -2.427472    -1.771582      21.01
 O      -2.175778    -3.337127    -1.973263     200.53
 H      -2.710554    -4.254820    -2.097812      15.43
 C      -3.623247    -3.534847     0.027577      87.37
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 H      -2.785314    -4.005182     0.412932      21.18
 O      -4.213220    -2.842183     1.017920     359.79
 H      -3.628278    -2.819484     1.943907      20.81
 C      -4.539156    -4.765471    -0.477332     101.65
 O      -3.910485    -5.459663    -1.677995     323.24
 H      -3.373728    -6.125206    -1.275908      31.25
 H      -5.531310    -4.649540    -0.736114      28.39
 H      -4.410014    -5.431915     0.466477      27.59
55
name = lig-etoh-frame_25
 C       2.701718     1.403606    -2.090681      51.70
 H       1.920727     1.858649    -2.683211      18.81
 C       3.407991     0.757012     0.208009      43.92
 H       3.376853     1.192742     1.281324      16.85
 C       3.926983    -0.442694    -0.179597      12.71
 O       4.501506    -1.242451     0.696871     217.81
 C       5.666203    -2.111112     0.593615     103.97
 H       5.299375    -3.144122     0.464773      24.50
 H       6.205140    -1.894115     1.550731      25.27
 H       6.348379    -1.750486    -0.293875      24.36
 C       4.025958    -0.760325    -1.616396       3.89
 O       4.636755    -1.844852    -2.322201     258.61
 H       4.302520    -2.756029    -2.430769      26.15
 C       3.267542     0.239146    -2.512825      53.44
 H       3.656244     0.077036    -3.589621      26.65
 C       2.702977     1.601949    -0.646966      50.57
 C       2.166213     2.978135     0.067058     109.47
 H       2.454444     3.811631    -0.655696      21.43
 O       2.384755     3.377985     1.392601     288.77
 H       3.423422     3.591265     1.365796      26.93
 C       0.599345     3.132912    -0.257771      51.60
 H       0.536724     2.933992    -1.351834      19.73
 C       0.008930     4.548881     0.327803      87.39
 O       0.813664     5.664097    -0.356783     224.92
 H       0.709243     5.635902    -1.484343      23.75
 H       0.274992     4.654631     1.462553      23.38
 H      -1.070813     4.689353     0.107732      23.43
 C      -0.902992    -1.350817    -0.424368      21.34
 H      -0.474256    -2.398437    -0.460294      15.71
 C      -3.049721    -0.000433    -0.838767      38.23
 H      -4.005968    -0.386548    -0.974569      21.47
 C      -2.389586     1.214081    -0.400533      10.92
 O      -3.032809     2.472043    -0.336427     232.80
 C      -3.698805     2.661260     0.944648      80.26
 H      -4.159024     1.710324     1.364509      23.74
 H      -2.705576     3.208989     1.704787      20.77
 H      -4.398795     3.621601     1.078768      23.17
 C      -1.043028     1.118571     0.017727       7.62
 O      -0.373090     2.236501     0.559125     185.16
 C      -0.345688    -0.086185    -0.100557      27.65
 H       0.961256    -0.114264    -0.100397      12.88
 C      -2.324776    -1.246666    -0.878503      10.19
 C      -3.127311    -2.479482    -1.099099      75.33
 H      -3.957182    -1.976172    -1.801336      19.83
 O      -2.211885    -3.349821    -1.950973     216.41
 H      -2.601699    -4.198047    -1.971731      20.06
 C      -3.599981    -3.549780     0.009489      78.31
 H      -2.578401    -4.086704     0.347377      18.33
 O      -4.233507    -2.834991     1.011513     396.64
 H      -3.682904    -2.792720     1.758972      28.32
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 C      -4.527570    -4.799894    -0.410705      96.19
 O      -3.963540    -5.410143    -1.695228     322.71
 H      -3.346856    -6.013487    -0.986756      22.53
 H      -5.631310    -4.596022    -0.711064      25.70
 H      -4.639241    -5.661037     0.256279      27.91
55
name = lig-etoh-frame_26
 C       2.757602     1.415091    -2.095487      35.85
 H       1.828325     1.863980    -2.580629      15.65
 C       3.444190     0.782236     0.199761      54.66
 H       3.112383     1.098565     1.180885      19.86
 C       3.979332    -0.455960    -0.220035      19.17
 O       4.501325    -1.261963     0.679164     248.90
 C       5.650213    -2.043626     0.610502     126.13
 H       5.448158    -3.102989     0.428588      26.05
 H       6.328661    -1.968324     1.477330      26.80
 H       6.380467    -1.900838    -0.252580      25.65
 C       4.010454    -0.793729    -1.626368      12.97
 O       4.605060    -1.776231    -2.318486     213.33
 H       4.206036    -2.829223    -2.259040      22.17
 C       3.336422     0.167011    -2.538350      30.26
 H       3.278370     0.099611    -3.621104      26.13
 C       2.671965     1.578232    -0.579794      53.08
 C       2.127668     3.010538     0.024087     102.37
 H       2.537756     3.693150    -0.810017      23.72
 O       2.406584     3.352194     1.347433     322.95
 H       3.293372     3.651758     1.409974      31.67
 C       0.514704     3.122794    -0.231800      76.16
 H       0.492988     3.101331    -1.333261      21.38
 C       0.004378     4.601092     0.245156     103.08
 O       0.884118     5.651710    -0.361287     293.08
 H       0.760034     5.554919    -1.248814      33.53
 H       0.059462     4.578283     1.284947      27.43
 H      -1.128657     4.683989     0.214312      25.08
 C      -0.947963    -1.275113    -0.378628      41.77
 H      -0.443669    -2.202171    -0.461896      16.68
 C      -2.892126    -0.018220    -0.767243      36.70
 H      -4.143995     0.037610    -0.753008      17.28
 C      -2.394265     1.205616    -0.417083       4.88
 O      -3.028200     2.512476    -0.362675     245.93
 C      -3.726456     2.682379     0.965847     117.90
 H      -4.245575     1.977971     1.663257      25.79
 H      -3.074430     2.925182     1.604456      31.61
 H      -4.607182     3.345379     1.132955      26.26
 C      -1.015103     1.096526     0.031815      -3.87
 O      -0.344775     2.237109     0.544570     208.49
 C      -0.252958    -0.119300    -0.093962      42.20
 H       0.704054    -0.024908     0.149460      17.95
 C      -2.281762    -1.284641    -0.831238      32.82
 C      -3.122008    -2.525426    -1.132030      87.04
 H      -3.894085    -1.950692    -1.639894      22.84
 O      -2.243482    -3.339232    -1.937594     224.71
 H      -2.665473    -4.270631    -1.943796      18.98
 C      -3.557068    -3.575396    -0.014583     101.25
 H      -2.598457    -3.953247     0.269877      23.64
 O      -4.286301    -2.820906     1.028232     356.40
 H      -3.539049    -2.688482     1.788899      23.12
 C      -4.537672    -4.804143    -0.398976      95.95
 O      -3.995806    -5.383952    -1.657770     334.70
 H      -3.312087    -5.959931    -1.357288      31.54
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 H      -5.462124    -4.257819    -0.624423      27.43
 H      -4.759543    -5.728876     0.260112      26.22
55
name = lig-etoh-frame_27
 C       2.765995     1.381145    -2.016401      65.65
 H       2.131822     1.926117    -2.699825      17.54
 C       3.440034     0.799025     0.229861      45.52
 H       3.276773     0.753802     1.367713      18.36
 C       4.048822    -0.461392    -0.336725      17.00
 O       4.501863    -1.300119     0.730004     239.36
 C       5.685017    -2.006705     0.598923     117.95
 H       5.359483    -3.079062     0.603261      25.59
 H       6.318583    -1.966899     1.572188      25.80
 H       6.301469    -1.739770    -0.284290      26.29
 C       3.927896    -0.739283    -1.666923      36.91
 O       4.596856    -1.761903    -2.318435     301.90
 H       4.227276    -2.513835    -2.001225      31.20
 C       3.395245     0.138934    -2.545139      11.67
 H       3.022565    -0.132945    -3.564299      19.60
 C       2.655461     1.625628    -0.597689      52.80
 C       2.033497     2.997085    -0.084605     108.15
 H       2.672971     3.719181    -0.737908      24.25
 O       2.431039     3.317681     1.314591     266.12
 H       3.390045     3.759943     1.504820      29.16
 C       0.449310     3.164121    -0.194388      86.16
 H       0.170567     3.093903    -1.301552      21.65
 C       0.026977     4.624749     0.151001     106.41
 O       0.927135     5.628614    -0.323415     252.95
 H       0.792799     5.570417    -1.441805      24.96
 H       0.120013     4.602737     1.328272      25.55
 H      -1.041635     4.751504    -0.023498      25.85
 C      -0.973741    -1.243993    -0.366749      50.83
 H      -0.297436    -2.137564    -0.392276      16.74
 C      -2.870644    -0.033526    -0.699810      45.17
 H      -3.824796     0.307142    -0.760871      19.11
 C      -2.322689     1.225635    -0.396916      -6.14
 O      -3.054257     2.511075    -0.369221     193.72
 C      -3.786519     2.696997     1.004656      59.13
 H      -4.176828     1.722981     1.441914      24.29
 H      -2.832663     3.016331     1.915703      21.72
 H      -4.688715     3.404104     0.722569      22.55
 C      -0.959150     1.109245     0.017915       4.89
 O      -0.317105     2.229096     0.530591     222.34
 C      -0.217771    -0.107347    -0.065966      33.12
 H       0.924295    -0.030596     0.467401      13.42
 C      -2.246120    -1.299543    -0.726193      43.03
 C      -3.104426    -2.586917    -1.170596      69.58
 H      -4.151435    -2.270591    -1.692763      21.12
 O      -2.264023    -3.335934    -1.953553     237.05
 H      -2.788725    -4.223899    -2.082691      17.60
 C      -3.549802    -3.572834    -0.001530      88.10
 H      -2.523415    -3.926834     0.443474      20.45
 O      -4.317229    -2.819741     1.060404     340.04
 H      -3.580564    -2.555460     1.723112      24.07
 C      -4.527356    -4.766900    -0.417371      91.06
 O      -4.030185    -5.366531    -1.627389     326.46
 H      -3.292705    -6.040867    -1.611287      29.64
 H      -5.395622    -4.077364    -0.654287      28.08
 H      -4.684366    -5.429745     0.400758      27.09
55
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name = lig-etoh-frame_28
 C       2.759481     1.304213    -1.947788      68.00
 H       2.556152     2.042654    -2.809067      26.42
 C       3.418804     0.747630     0.260198      35.32
 H       3.664063     0.536650     1.320149      20.72
 C       4.087960    -0.399420    -0.350813      -2.19
 O       4.474119    -1.306797     0.773262     187.93
 C       5.752624    -2.028605     0.609361     108.80
 H       5.450752    -3.069763     0.617833      26.48
 H       6.252230    -1.791849     1.528821      27.21
 H       6.224759    -1.535194    -0.363714      25.26
 C       3.890580    -0.701037    -1.727410      31.70
 O       4.600343    -1.771328    -2.318213     210.48
 H       4.287647    -2.596754    -1.750166      25.93
 C       3.353958     0.225119    -2.557621      35.94
 H       3.064174    -0.373626    -3.457511      18.93
 C       2.667784     1.693373    -0.630492      43.24
 C       1.978083     2.975878    -0.173439     115.88
 H       2.450029     3.807027    -0.707732      20.53
 O       2.444895     3.278131     1.290864     278.81
 H       3.357538     3.653635     1.254110      28.53
 C       0.409435     3.220262    -0.227652      81.28
 H      -0.007346     2.980836    -1.198899      21.89
 C       0.060985     4.623231     0.138133     117.27
 O       0.954978     5.605469    -0.323887     279.32
 H       0.954596     5.769029    -1.270297      30.33
 H       0.166076     4.759863     1.153995      27.34
 H      -0.936505     4.885974    -0.317250      24.64
 C      -0.872052    -1.272567    -0.350483      40.58
 H      -0.317438    -2.206555    -0.295683      21.77
 C      -2.901765     0.000894    -0.632198      25.58
 H      -4.091234     0.163557    -1.050680      20.62
 C      -2.207375     1.248802    -0.353018      -2.38
 O      -3.077157     2.463620    -0.350066     167.77
 C      -3.806914     2.699969     1.060991      91.64
 H      -4.076637     1.643063     0.982151      24.21
 H      -3.232534     3.157437     1.661629      28.71
 H      -4.399761     3.397080     0.450508      24.06
 C      -0.870855     1.157835    -0.014433      20.47
 O      -0.288404     2.229991     0.552611     233.69
 C      -0.198100    -0.047581     0.000231      37.81
 H       0.741695    -0.257143     0.502680      18.37
 C      -2.327276    -1.306181    -0.642874      28.05
 C      -3.119234    -2.615153    -1.161818      76.23
 H      -4.055199    -2.585505    -1.676858      20.84
 O      -2.262510    -3.360883    -2.016092     288.90
 H      -2.795152    -4.075729    -2.280005      22.17
 C      -3.534937    -3.545242     0.061668      98.48
 H      -2.682027    -3.964403     0.633589      18.68
 O      -4.331927    -2.827591     1.078910     348.88
 H      -3.697402    -2.540659     1.706878      27.74
 C      -4.471749    -4.664157    -0.432222      89.52
 O      -4.076176    -5.355382    -1.628672     272.86
 H      -3.362990    -6.182986    -1.479247      26.71
 H      -5.469008    -4.247461    -0.799116      26.81
 H      -4.622067    -5.193950     0.592602      25.64
55
name = lig-etoh-frame_29
 C       2.722928     1.318422    -1.965289      75.84
 H       2.691932     2.164053    -2.615645      27.24
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 C       3.401440     0.681820     0.247006      52.72
 H       3.727578     0.790091     1.303228      22.45
 C       4.079752    -0.328012    -0.290724      13.51
 O       4.438306    -1.295548     0.775629     170.39
 C       5.792000    -2.026596     0.613988     111.12
 H       5.742771    -3.144493     0.495804      26.88
 H       6.399829    -1.609096     1.527203      25.58
 H       6.268084    -1.738583    -0.233786      29.60
 C       3.936225    -0.705186    -1.744228      12.03
 O       4.578645    -1.801953    -2.309286     177.84
 H       4.632915    -2.666454    -1.631244      23.41
 C       3.286537     0.254230    -2.576721      43.27
 H       3.181963    -0.100277    -3.592515      19.41
 C       2.717096     1.708800    -0.604036      41.14
 C       1.965584     2.974973    -0.205702     101.34
 H       2.145019     3.982182    -0.860493      16.52
 O       2.430625     3.228661     1.240395     281.82
 H       3.351517     3.506539     1.057654      27.07
 C       0.405172     3.213036    -0.298456      63.46
 H       0.033063     2.979091    -1.363887      19.39
 C       0.076329     4.644077     0.129659     106.77
 O       1.014182     5.616583    -0.326517     271.97
 H       0.971672     5.795792    -1.318493      29.34
 H       0.006640     4.820277     1.284881      24.36
 H      -0.899350     4.921953    -0.180403      24.91
 C      -0.802007    -1.302507    -0.331021      28.36
 H      -0.347616    -2.291465    -0.202648      21.21
 C      -2.985018     0.047379    -0.600728      30.03
 H      -3.854146    -0.088918    -1.048197      22.38
 C      -2.179943     1.252271    -0.319831      -3.31
 O      -3.041783     2.390672    -0.328807     167.33
 C      -3.827799     2.673196     0.980520      71.44
 H      -4.325809     1.650159     1.128643      22.71
 H      -3.214740     3.401862     1.943535      21.15
 H      -4.535354     3.436731     0.596629      23.74
 C      -0.784999     1.225304    -0.038277      17.13
 O      -0.245514     2.269626     0.623821     216.09
 C      -0.213225    -0.074084     0.055764      19.75
 H       0.840482    -0.255979     0.539385      16.67
 C      -2.392873    -1.290039    -0.596589     -11.91
 C      -3.110396    -2.629251    -1.088830      62.23
 H      -4.089868    -2.393457    -1.710525      20.32
 O      -2.231279    -3.383138    -2.092116     221.37
 H      -2.856501    -4.110373    -2.550683      18.77
 C      -3.524733    -3.496790     0.131484     105.40
 H      -2.686798    -4.037481     0.667469      19.92
 O      -4.352957    -2.838070     1.078209     316.03
 H      -3.670616    -2.535733     1.880143      22.86
 C      -4.437756    -4.558842    -0.414664     112.21
 O      -4.103237    -5.378271    -1.636026     325.50
 H      -3.636791    -6.014693    -1.204848      32.63
 H      -5.447972    -4.309722    -0.759277      27.64
 H      -4.623681    -5.206091     0.401376      28.20
55
name = lig-etoh-frame_30
 C       2.681663     1.433861    -1.990582      51.03
 H       2.408607     2.367799    -2.579357      17.89
 C       3.356529     0.728965     0.253298      44.76
 H       3.458757     1.219106     1.265497      19.89
 C       4.069196    -0.366668    -0.270296      19.05
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 O       4.433299    -1.297806     0.743115     190.88
 C       5.806678    -1.988522     0.644468     110.93
 H       5.826305    -3.078842     0.684451      26.91
 H       6.398604    -1.713773     1.434072      28.46
 H       6.472179    -1.785083    -0.387719      26.03
 C       4.000039    -0.700702    -1.708846      21.35
 O       4.558460    -1.847099    -2.290998     244.57
 H       4.839270    -2.436113    -1.719835      27.96
 C       3.255339     0.178926    -2.591534      45.90
 H       3.331236     0.434244    -3.745077      20.78
 C       2.767697     1.662035    -0.584830      21.14
 C       1.974505     3.008646    -0.203534     109.22
 H       2.253489     3.794176    -0.892054      19.10
 O       2.392273     3.186486     1.156695     269.92
 H       3.450976     3.411806     1.136213      26.03
 C       0.434561     3.163306    -0.353349      74.33
 H       0.190697     3.064427    -1.384119      18.44
 C       0.074766     4.686915     0.147163      91.65
 O       1.087770     5.653896    -0.330067     255.21
 H       0.839427     5.641677    -1.404791      24.75
 H      -0.034911     4.611250     1.203626      25.75
 H      -1.036980     4.907111    -0.110224      22.83
 C      -0.853214    -1.315603    -0.305085      43.39
 H      -0.331752    -2.292475    -0.119104      21.03
 C      -2.980935     0.028114    -0.574653      25.27
 H      -4.146826     0.011633    -1.082952      20.09
 C      -2.228877     1.224166    -0.295492      -0.31
 O      -2.984100     2.340718    -0.287432     245.50
 C      -3.831905     2.671955     0.883338     119.17
 H      -4.440063     1.948705     1.521962      25.21
 H      -3.381644     2.929226     1.701036      28.96
 H      -4.756668     3.344057     0.812099      25.38
 C      -0.769577     1.240103    -0.032315      -2.31
 O      -0.195138     2.338900     0.696042     208.54
 C      -0.204772    -0.156050     0.103453       6.07
 H       0.917465     0.009347     0.449362      15.49
 C      -2.351006    -1.251839    -0.578710      10.94
 C      -3.082721    -2.601205    -1.028370      61.28
 H      -3.916585    -2.093544    -1.498654      21.49
 O      -2.210851    -3.391329    -2.152272     223.79
 H      -2.828023    -4.024820    -2.581622      21.19
 C      -3.508388    -3.467445     0.165155     108.72
 H      -2.573785    -4.004617     0.570890      19.70
 O      -4.363368    -2.826684     1.104230     341.54
 H      -3.794110    -2.645423     1.838352      28.87
 C      -4.458044    -4.511513    -0.410864      87.58
 O      -4.119820    -5.393436    -1.626901     255.54
 H      -3.660223    -6.111238    -1.022321      26.05
 H      -5.496540    -3.947709    -0.585727      26.59
 H      -4.647054    -5.416516     0.285792      24.77
55
name = lig-etoh-frame_31
 C       2.684145     1.509926    -2.022007      42.11
 H       2.071118     2.201514    -2.620049      17.72
 C       3.326806     0.827426     0.277074      21.66
 H       3.217344     1.212595     1.270808      18.13
 C       4.036976    -0.441046    -0.269569       9.82
 O       4.473434    -1.325249     0.697763     228.99
 C       5.820380    -1.936976     0.633634     109.89
 H       5.565183    -3.011447     0.924972      24.29
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 H       6.459844    -1.622583     1.608331      24.64
 H       6.316908    -1.720069    -0.193936      28.80
 C       4.036899    -0.680651    -1.671851       5.89
 O       4.530929    -1.869216    -2.287599     173.73
 H       5.113248    -2.418332    -1.537183      21.64
 C       3.232794     0.190882    -2.588946      53.98
 H       3.548442     0.435824    -3.547159      27.16
 C       2.743424     1.640697    -0.650943      16.28
 C       2.024010     3.001729    -0.191780     121.24
 H       2.701949     3.677483    -0.938986      21.66
 O       2.365985     3.174820     1.095516     348.10
 H       3.235067     3.394907     1.296556      32.54
 C       0.501869     3.164850    -0.335470      75.66
 H       0.168149     2.962874    -1.435554      18.86
 C       0.070279     4.700453     0.145194      91.86
 O       1.116921     5.681315    -0.344424     271.77
 H       0.996678     5.665097    -1.261215      31.32
 H       0.185200     4.506971     1.269070      25.49
 H      -0.916488     4.917055    -0.204146      24.83
 C      -0.956643    -1.319103    -0.253594      47.53
 H      -0.453947    -2.234961    -0.148247      20.10
 C      -2.974254    -0.034022    -0.589176      44.37
 H      -3.904365     0.281548    -0.729212      22.08
 C      -2.260160     1.158389    -0.255805       4.51
 O      -2.959437     2.345604    -0.235071     242.38
 C      -3.886814     2.641946     0.808279      89.60
 H      -4.352443     1.864838     1.460802      24.26
 H      -2.953409     2.913627     1.797801      19.65
 H      -4.642084     3.363637     0.566268      24.80
 C      -0.832987     1.166497     0.030624       1.24
 O      -0.165130     2.382797     0.712866     187.02
 C      -0.181500    -0.148367     0.126265      14.26
 H       0.862128    -0.075297     0.372519      17.04
 C      -2.236872    -1.239870    -0.584482      40.21
 C      -3.010758    -2.511320    -0.991459      58.92
 H      -3.961105    -2.066251    -1.442690      20.80
 O      -2.214701    -3.361327    -2.166819     223.09
 H      -2.866145    -3.995600    -2.469294      21.58
 C      -3.478750    -3.484598     0.146168     101.47
 H      -2.570642    -3.859270     0.590955      21.04
 O      -4.368986    -2.805468     1.137955     309.50
 H      -3.779828    -2.675366     1.939336      25.86
 C      -4.531442    -4.526867    -0.409944      95.79
 O      -4.128452    -5.391499    -1.591106     279.14
 H      -3.600697    -6.233275    -1.200431      27.59
 H      -5.316751    -3.807380    -0.530736      30.15
 H      -4.727972    -5.237104     0.355715      27.03
55
name = lig-etoh-frame_32
 C       2.708830     1.463456    -2.094976      50.44
 H       1.958736     1.946124    -2.724632      18.95
 C       3.346546     0.853784     0.257673      22.84
 H       3.115067     0.892646     1.389274      17.30
 C       3.963107    -0.443179    -0.245952      -0.51
 O       4.524839    -1.356492     0.658444     235.12
 C       5.806992    -1.897197     0.706616     110.77
 H       5.484414    -2.928349     0.889962      23.91
 H       6.338315    -1.438226     1.464997      26.85
 H       6.387213    -1.673012    -0.367118      24.46
 C       4.023783    -0.649892    -1.666846       1.18
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 O       4.508659    -1.883104    -2.260437     172.87
 H       5.246494    -2.268763    -1.613812      21.85
 C       3.248730     0.287482    -2.525218      53.48
 H       3.676292     0.047293    -3.638103      25.65
 C       2.649447     1.676232    -0.724453      38.74
 C       2.139369     2.965122    -0.247244     132.82
 H       2.654285     3.679744    -0.779905      23.96
 O       2.330026     3.188806     1.119330     294.77
 H       3.297722     3.537907     1.332896      28.08
 C       0.563371     3.218116    -0.310168      72.66
 H       0.148855     2.858607    -1.195961      23.12
 C       0.137118     4.672068     0.124253      97.08
 O       1.108518     5.696381    -0.322253     215.65
 H       1.199278     5.752888    -1.444593      24.87
 H       0.354906     4.713600     1.212436      25.45
 H      -0.877526     4.977459    -0.249760      24.30
 C      -0.943506    -1.285887    -0.159232      34.91
 H      -0.531747    -2.359034    -0.233408      13.92
 C      -2.908032    -0.051515    -0.592151      45.02
 H      -4.108008     0.256211    -0.520905      18.38
 C      -2.260924     1.091116    -0.199245      11.03
 O      -2.947974     2.362155    -0.214790     235.14
 C      -3.866260     2.614143     0.845992      99.46
 H      -4.315953     1.580083     1.035791      23.63
 H      -3.273998     3.109537     1.402606      27.82
 H      -4.383084     3.484969     0.248799      22.91
 C      -0.896191     1.070913     0.154420       7.83
 O      -0.167964     2.369550     0.674784     149.89
 C      -0.207656    -0.089442     0.120011      46.31
 H       0.978488    -0.405551     0.369639      14.65
 C      -2.221943    -1.267216    -0.630320      51.01
 C      -2.953474    -2.429047    -0.996359      79.29
 H      -3.935977    -2.253702    -1.481156      22.75
 O      -2.243991    -3.289697    -2.132898     185.86
 H      -2.968617    -4.074709    -2.249499      18.77
 C      -3.458067    -3.505858     0.104862      83.05
 H      -2.552236    -3.876436     0.785708      20.47
 O      -4.356909    -2.782963     1.165694     282.61
 H      -3.688118    -2.713329     2.013431      23.02
 C      -4.552610    -4.569115    -0.399601      75.73
 O      -4.143315    -5.377208    -1.549234     325.25
 H      -3.638434    -6.063469    -1.309754      34.47
 H      -5.425057    -3.820423    -0.834719      27.71
 H      -4.913520    -5.047292     0.581286      26.72
55
name = lig-etoh-frame_33
 C       2.690953     1.394586    -2.170417      36.91
 H       2.050017     1.885267    -2.939335      19.68
 C       3.359868     0.806647     0.197746      55.48
 H       3.177722     0.704947     1.221204      20.65
 C       3.897818    -0.389491    -0.232185      13.91
 O       4.516622    -1.359392     0.630756     249.00
 C       5.804982    -1.857782     0.723454     121.51
 H       5.816060    -2.993432     0.855377      25.27
 H       6.421867    -1.226433     1.530715      25.23
 H       6.366069    -1.851149    -0.132775      28.53
 C       3.971066    -0.618133    -1.655319       8.07
 O       4.486006    -1.862990    -2.221154     230.63
 H       5.188731    -2.151550    -1.787287      26.69
 C       3.385482     0.297995    -2.513192      20.97
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 H       3.268608    -0.211297    -3.434131      23.66
 C       2.595129     1.681173    -0.740097      70.05
 C       2.195483     2.960989    -0.283121     125.36
 H       2.524244     4.014095    -0.836897      21.29
 O       2.328748     3.216252     1.203526     268.85
 H       3.262134     3.632994     1.235800      29.77
 C       0.601450     3.250113    -0.288813      59.37
 H       0.131270     2.920639    -1.299329      21.03
 C       0.248824     4.655709     0.082351     112.12
 O       1.096418     5.715045    -0.323861     276.54
 H       1.143611     5.696326    -1.265980      32.07
 H       0.261084     4.837847     1.161322      26.65
 H      -0.814822     4.884302    -0.141569      25.71
 C      -0.870569    -1.282645    -0.086673      36.20
 H      -0.420070    -2.219191    -0.188630      15.95
 C      -2.908935    -0.026687    -0.580131      47.28
 H      -3.912466    -0.243153    -0.642643      20.48
 C      -2.251309     1.100054    -0.130279      14.10
 O      -2.892575     2.341998    -0.240815     223.12
 C      -3.858978     2.597567     0.826948      92.83
 H      -4.490872     1.689658     0.829387      23.57
 H      -3.476349     3.436643     1.848505      21.20
 H      -4.460704     3.287417     0.299849      25.52
 C      -0.908863     1.078308     0.297687       3.88
 O      -0.197565     2.309226     0.628697     186.19
 C      -0.190633    -0.124745     0.124539      58.03
 H       0.732474    -0.275194     0.353880      19.91
 C      -2.249226    -1.264204    -0.662319      23.36
 C      -2.963295    -2.475446    -1.047140      88.14
 H      -3.903995    -2.158525    -1.529757      22.17
 O      -2.299752    -3.209342    -2.065250     272.61
 H      -2.791951    -4.014218    -2.061423      21.93
 C      -3.448309    -3.505218     0.110272     102.17
 H      -2.718881    -4.002597     0.644476      24.61
 O      -4.317272    -2.769816     1.182993     342.52
 H      -3.698819    -2.726107     1.850270      29.96
 C      -4.552573    -4.560655    -0.396745     100.77
 O      -4.176949    -5.349787    -1.509115     295.27
 H      -3.463572    -6.096640    -1.156990      27.76
 H      -5.347006    -4.139328    -0.944763      28.62
 H      -4.971187    -4.987476     0.505516      28.33
55
name = lig-etoh-frame_34
 C       2.634887     1.364144    -2.185820      75.45
 H       2.273471     1.944976    -3.026146      26.07
 C       3.318710     0.763412     0.123192      43.79
 H       3.256994     0.913212     1.268816      19.01
 C       3.910356    -0.375438    -0.275655      22.81
 O       4.446439    -1.349629     0.620436     221.00
 C       5.839228    -1.820743     0.748514     115.97
 H       6.047146    -2.855269     1.082612      26.49
 H       6.355561    -1.281656     1.483458      27.89
 H       6.524570    -1.801623    -0.273741      25.97
 C       3.949101    -0.635723    -1.610103      21.57
 O       4.427860    -1.806281    -2.188269     168.23
 H       5.397792    -2.146742    -1.754790      23.75
 C       3.522895     0.223112    -2.564585      58.24
 H       2.968558    -0.231692    -3.499542      17.78
 C       2.626422     1.634059    -0.771265      38.58
 C       2.141583     3.060795    -0.247971     106.68
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 H       2.475549     3.824511    -0.810408      22.85
 O       2.364888     3.246064     1.270293     294.94
 H       3.232577     3.624775     1.366157      29.05
 C       0.613522     3.200242    -0.324188      63.41
 H       0.306078     3.201155    -1.350729      20.91
 C       0.317731     4.663744     0.090563     105.91
 O       1.094846     5.739573    -0.335852     264.01
 H       1.028593     5.693291    -1.391602      27.15
 H       0.138958     4.691080     1.232176      24.64
 H      -0.761065     4.728629    -0.217375      24.01
 C      -0.867071    -1.325554    -0.095406      45.00
 H      -0.125790    -2.212477    -0.056907      14.38
 C      -2.916065    -0.053938    -0.567074      31.14
 H      -4.018137    -0.363271    -0.919256      17.78
 C      -2.235861     1.156215    -0.055423       7.00
 O      -2.828001     2.327680    -0.255128     250.49
 C      -3.862563     2.645659     0.803094     113.46
 H      -4.586160     1.820769     1.090211      25.28
 H      -3.778074     2.878988     1.769197      27.83
 H      -4.765125     3.263905     0.359238      24.93
 C      -0.876594     1.139807     0.388809       6.20
 O      -0.229753     2.248569     0.603273     200.49
 C      -0.185217    -0.156512     0.164500      24.18
 H       1.059306     0.018933     0.492711      13.76
 C      -2.199840    -1.234777    -0.625415      16.26
 C      -3.045217    -2.553288    -1.079098      64.15
 H      -3.966882    -1.974474    -1.469274      22.50
 O      -2.329831    -3.147556    -2.009797     252.08
 H      -2.631090    -4.113151    -2.070763      18.84
 C      -3.513339    -3.475721     0.122324      84.89
 H      -2.616869    -4.223861     0.501750      19.65
 O      -4.266565    -2.774223     1.160418     327.14
 H      -3.501039    -2.644468     1.938532      21.91
 C      -4.539117    -4.501331    -0.397749      91.66
 O      -4.168251    -5.375497    -1.472368     306.05
 H      -3.442727    -5.960435    -1.049517      30.83
 H      -5.564108    -4.018562    -0.883420      25.90
 H      -4.852192    -5.198692     0.439682      26.71
55
name = lig-etoh-frame_35
 C       2.646336     1.304076    -2.168914      62.83
 H       2.399039     2.086274    -2.942342      24.82
 C       3.240310     0.766847     0.110619      53.05
 H       3.373103     1.252188     1.055320      21.15
 C       3.984519    -0.409786    -0.296845      21.75
 O       4.375640    -1.355364     0.633543     206.03
 C       5.888807    -1.774892     0.731831     107.19
 H       5.835910    -2.761441     1.241966      25.47
 H       6.325756    -1.071238     1.572632      25.16
 H       6.368546    -1.607377    -0.167126      28.32
 C       3.972212    -0.698067    -1.623129      18.32
 O       4.394127    -1.782610    -2.151500     214.06
 H       5.286629    -2.091069    -1.786814      25.05
 C       3.513877     0.204492    -2.653740      39.56
 H       3.211450    -0.191969    -3.645004      19.43
 C       2.677640     1.632903    -0.815795      20.91
 C       2.055263     3.081013    -0.141971      93.86
 H       2.662447     3.838253    -0.901768      18.77
 O       2.403918     3.273448     1.298794     288.86
 H       3.413365     3.606734     1.528988      26.00
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 C       0.624621     3.152195    -0.365097      64.26
 H       0.393006     3.178955    -1.475804      18.75
 C       0.278069     4.648304     0.157003     100.74
 O       1.105642     5.760975    -0.375803     220.63
 H       0.907648     5.802433    -1.421485      26.81
 H       0.270970     4.577490     1.194583      26.87
 H      -0.687697     4.754010    -0.386256      23.05
 C      -0.835275    -1.375736    -0.135264      42.65
 H      -0.224256    -2.240144    -0.011339      15.44
 C      -2.913482    -0.082854    -0.541859      39.05
 H      -3.845358     0.147326    -1.057031      19.70
 C      -2.228314     1.143498    -0.004601      11.08
 O      -2.813192     2.375148    -0.232285     237.27
 C      -3.949544     2.668284     0.733158      84.67
 H      -4.426258     1.682361     1.062952      25.30
 H      -3.479721     2.650159     1.989457      22.13
 H      -4.658548     3.401723     0.400588      25.32
 C      -0.861068     1.106185     0.379205       7.58
 O      -0.213456     2.269717     0.599632     201.61
 C      -0.143947    -0.113821     0.264774      29.02
 H       0.790712    -0.024775     0.442120      18.17
 C      -2.156077    -1.269926    -0.556007      28.92
 C      -3.152889    -2.517290    -1.017641      61.75
 H      -4.058161    -2.088691    -1.420947      25.35
 O      -2.321485    -3.145476    -2.013712     248.14
 H      -2.470537    -4.157209    -2.201718      18.75
 C      -3.579507    -3.474333     0.115063     107.99
 H      -2.733332    -3.979509     0.361200      23.64
 O      -4.187494    -2.786532     1.147122     385.07
 H      -3.494041    -2.535202     1.806881      26.25
 C      -4.596055    -4.449450    -0.393947     104.91
 O      -4.123310    -5.413707    -1.449164     350.50
 H      -3.479157    -5.921502    -1.023083      34.63
 H      -5.440748    -3.884091    -0.554917      30.54
 H      -4.685906    -5.226153     0.384938      26.86
55
name = lig-etoh-frame_36
 C       2.717727     1.259697    -2.192342      71.91
 H       2.361153     2.081425    -2.779911      26.58
 C       3.214335     0.770248     0.111490      65.31
 H       3.438451     1.339888     1.047933      22.05
 C       4.023997    -0.398588    -0.268038       7.74
 O       4.342023    -1.377888     0.664550     197.49
 C       5.871744    -1.690036     0.772281      99.37
 H       5.649961    -2.724534     1.144702      24.09
 H       6.202574    -0.915636     1.449135      26.00
 H       6.371478    -1.547052    -0.285809      26.65
 C       3.974487    -0.674531    -1.700007       9.82
 O       4.402786    -1.862158    -2.152696     227.79
 H       5.158000    -2.171687    -1.774753      26.21
 C       3.419625     0.217913    -2.694219      32.33
 H       3.630103    -0.137707    -3.802365      17.76
 C       2.703193     1.670539    -0.817700      24.40
 C       2.083757     3.029514    -0.070752     122.44
 H       2.507884     3.765354    -0.626876      20.41
 O       2.445961     3.299605     1.311976     336.00
 H       3.378995     3.501658     1.321988      30.63
 C       0.603408     3.156877    -0.375415      68.22
 H       0.398084     2.864562    -1.420343      19.02
 C       0.195451     4.621474     0.157796      87.62
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 O       1.105527     5.764835    -0.412505     224.30
 H       0.911439     5.800427    -1.320269      30.33
 H       0.412081     4.633796     1.324518      23.86
 H      -0.785108     4.909428    -0.210726      23.20
 C      -0.769456    -1.355038    -0.148886      44.21
 H      -0.421582    -2.424964    -0.090303      18.14
 C      -2.849851    -0.028450    -0.490879      33.54
 H      -3.697187     0.434627    -1.077666      19.36
 C      -2.243548     1.083217     0.001607      -3.55
 O      -2.834441     2.448064    -0.190578     183.11
 C      -3.980050     2.620294     0.740943      97.60
 H      -4.450293     1.634382     0.633831      23.63
 H      -3.353387     2.910601     1.514100      24.14
 H      -4.496927     3.623298     0.410565      24.20
 C      -0.857632     1.045812     0.309141       9.37
 O      -0.165866     2.342813     0.604517     178.21
 C      -0.174367    -0.117971     0.347216      28.42
 H       1.086618    -0.191196     0.522241      13.34
 C      -2.205202    -1.352120    -0.496937      28.75
 C      -3.196953    -2.441045    -0.944952      59.40
 H      -4.172390    -2.146560    -1.503035      20.75
 O      -2.296872    -3.163567    -2.047973     222.71
 H      -2.571584    -4.039353    -2.172922      21.98
 C      -3.607445    -3.467372     0.063882      92.10
 H      -2.545419    -3.922840     0.452919      16.68
 O      -4.141422    -2.784042     1.153208     365.42
 H      -3.371443    -2.523823     1.777476      22.33
 C      -4.627685    -4.478948    -0.367823      76.64
 O      -4.090199    -5.421498    -1.448982     278.45
 H      -3.383731    -6.032579    -0.824310      26.29
 H      -5.658114    -3.796604    -0.510510      26.28
 H      -4.817353    -5.046198     0.557139      27.08
55
name = lig-etoh-frame_37
 C       2.764358     1.324060    -2.207820      69.08
 H       2.240498     2.023817    -2.914120      20.60
 C       3.272292     0.774809     0.132177      39.84
 H       3.366057     1.037992     1.218205      19.93
 C       3.989175    -0.346978    -0.276446       3.73
 O       4.341351    -1.393652     0.688682     218.22
 C       5.773611    -1.597277     0.792638     119.13
 H       5.889388    -2.652984     1.074733      26.21
 H       6.234520    -0.823549     1.480493      26.09
 H       6.315596    -1.665446    -0.164722      27.81
 C       3.973234    -0.623850    -1.738576      -1.28
 O       4.415689    -1.980612    -2.195754     129.68
 H       5.232374    -2.415864    -1.544899      20.75
 C       3.347541     0.167216    -2.720707      46.11
 H       3.955930     0.188386    -3.677576      23.12
 C       2.712698     1.690154    -0.774503      27.94
 C       2.145749     2.941714    -0.058211     112.84
 H       2.489679     3.993309    -0.605177      16.76
 O       2.471155     3.301393     1.311358     295.89
 H       3.474749     3.519515     1.190540      26.13
 C       0.565254     3.175221    -0.326407      71.55
 H       0.346828     2.725325    -1.300142      19.30
 C       0.141705     4.624259     0.119798      96.43
 O       1.082838     5.738618    -0.410572     200.40
 H       0.930201     5.690194    -1.539611      23.22
 H       0.378658     4.692189     1.109889      26.76
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 H      -0.962647     4.951257     0.168793      24.00
 C      -0.782078    -1.338894    -0.141870      42.28
 H      -0.445654    -2.404871    -0.196261      17.93
 C      -2.797002     0.008651    -0.464733      29.18
 H      -3.752024     0.205474    -1.067012      20.16
 C      -2.217997     1.120301    -0.004536       8.07
 O      -2.839434     2.479766    -0.170463     176.39
 C      -3.978345     2.582158     0.713892     101.10
 H      -4.786043     1.814036     0.505913      22.85
 H      -3.400525     3.133456     1.706834      20.17
 H      -4.414493     3.544504     0.366655      25.01
 C      -0.831203     1.080553     0.245495      -2.78
 O      -0.141545     2.381129     0.616697     180.38
 C      -0.144972    -0.212965     0.388424      32.53
 H       0.857815    -0.240923     0.629774      17.71
 C      -2.277951    -1.360629    -0.446988      17.47
 C      -3.178756    -2.397438    -0.959247      79.46
 H      -4.009375    -1.984946    -1.460269      21.41
 O      -2.283910    -3.162789    -2.072652     173.42
 H      -2.852965    -4.043294    -2.098847      17.00
 C      -3.551749    -3.470640     0.036993     115.20
 H      -2.729406    -3.976487     0.353408      21.89
 O      -4.137408    -2.766054     1.179922     340.19
 H      -3.279309    -2.642626     1.826490      20.81
 C      -4.665397    -4.527048    -0.334362      89.60
 O      -4.062190    -5.420605    -1.414986     331.24
 H      -3.513221    -5.954334    -0.874884      32.42
 H      -5.510607    -4.145242    -0.781801      29.05
 H      -5.023832    -4.931340     0.657439      27.21
55
name = lig-etoh-frame_38
 C       2.768040     1.457169    -2.189852      43.48
 H       2.278209     1.954789    -3.012450      18.96
 C       3.366641     0.784608     0.185227      34.32
 H       3.188082     0.722668     1.260041      18.80
 C       3.927438    -0.341311    -0.337930       1.15
 O       4.342870    -1.379761     0.686623     221.51
 C       5.675007    -1.530534     0.818149     125.42
 H       6.144749    -2.482938     1.262479      26.04
 H       6.293890    -0.839183     1.482378      26.61
 H       6.247913    -1.548400    -0.189125      27.02
 C       3.995569    -0.667178    -1.726230      -1.74
 O       4.438466    -2.066655    -2.227271     197.23
 H       4.946852    -2.465087    -1.494479      23.57
 C       3.341696     0.134465    -2.712285      53.56
 H       3.809898     0.319826    -3.690185      25.29
 C       2.723883     1.688905    -0.732213      29.99
 C       2.176749     2.944227    -0.120933     114.86
 H       2.456341     3.781098    -0.672726      22.89
 O       2.503474     3.271231     1.298186     279.31
 H       3.492607     3.621536     1.404172      27.28
 C       0.546231     3.176589    -0.254466      76.40
 H       0.274602     2.894826    -1.325411      20.50
 C       0.118527     4.665743     0.067251     104.31
 O       1.016045     5.682945    -0.436868     292.07
 H       1.064394     5.583880    -1.347761      32.17
 H       0.449761     4.639705     1.213955      24.64
 H      -0.943366     4.785196     0.193067      25.91
 C      -0.890778    -1.376050    -0.125463      53.64
 H      -0.258614    -2.245826    -0.217996      18.68
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 C      -2.816058    -0.030510    -0.483600      30.20
 H      -3.820265    -0.099529    -0.876954      22.02
 C      -2.138075     1.261146    -0.020889       4.04
 O      -2.825373     2.452505    -0.163574     246.25
 C      -3.964077     2.623059     0.695288     119.05
 H      -4.868669     1.983907     0.779723      25.32
 H      -3.890671     2.683847     1.829078      24.94
 H      -4.519007     3.512710     0.218660      24.93
 C      -0.755893     1.151024     0.224360       9.49
 O      -0.159026     2.355608     0.655079     224.43
 C      -0.156739    -0.271072     0.377178       9.99
 H       0.987963    -0.287506     0.802588      14.90
 C      -2.279869    -1.257016    -0.404941      33.04
 C      -3.095103    -2.407561    -1.035231      60.24
 H      -3.979322    -1.761918    -1.463215      20.50
 O      -2.311065    -3.160538    -2.075695     217.57
 H      -2.949081    -3.950179    -2.160134      18.35
 C      -3.553600    -3.469439     0.041953      72.79
 H      -2.627291    -4.220455     0.294572      16.66
 O      -4.139879    -2.759053     1.203370     338.80
 H      -3.464331    -2.669674     1.923540      24.13
 C      -4.665830    -4.560417    -0.325277      81.68
 O      -4.052364    -5.416760    -1.354562     288.42
 H      -3.402149    -6.072458    -0.894168      27.72
 H      -5.509700    -4.292489    -1.185381      23.81
 H      -5.008235    -5.056698     0.563832      26.94
55
name = lig-etoh-frame_39
 C       2.790774     1.506429    -2.139199      37.43
 H       2.348781     2.160709    -2.929167      15.52
 C       3.433525     0.801500     0.214113      43.85
 H       3.033757     0.637017     1.267402      17.06
 C       3.896073    -0.414155    -0.389500       7.69
 O       4.297497    -1.343423     0.663387     225.15
 C       5.698937    -1.487648     0.839708     112.83
 H       5.915673    -2.364825     1.418292      26.73
 H       6.122007    -0.625972     1.449354      26.58
 H       6.133916    -1.308505    -0.178744      27.03
 C       4.011095    -0.789790    -1.745230      14.01
 O       4.440980    -2.085558    -2.237883     239.50
 H       4.745747    -2.557379    -1.460374      22.81
 C       3.371197     0.195882    -2.637875      42.41
 H       3.357559     0.106488    -3.857885      24.23
 C       2.747006     1.687192    -0.711424      45.25
 C       2.154083     2.994007    -0.167890     102.13
 H       2.587967     3.786609    -0.969625      22.53
 O       2.534651     3.226522     1.278345     302.95
 H       3.407121     3.584705     1.469346      32.06
 C       0.554307     3.174910    -0.219619      78.00
 H       0.248200     3.099800    -1.247858      20.62
 C       0.152646     4.670405     0.102549     111.37
 O       0.930984     5.630673    -0.454411     263.60
 H       1.089945     5.488848    -1.527101      26.11
 H       0.371629     4.652877     1.125122      26.91
 H      -0.989286     4.715121    -0.148475      24.47
 C      -0.955047    -1.395477    -0.068935      48.40
 H      -0.238042    -2.281210    -0.222162      14.98
 C      -2.851486     0.020934    -0.487444      32.70
 H      -4.028697    -0.094106    -0.585611      22.74
 C      -2.077582     1.309123    -0.084257       3.91
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 O      -2.812766     2.422071    -0.145758     245.09
 C      -4.001780     2.698009     0.697972     103.38
 H      -4.746983     1.752449     0.628987      23.41
 H      -4.052504     2.359078     1.807070      23.41
 H      -4.499970     3.607101     0.243063      24.50
 C      -0.686136     1.179765     0.237445      21.09
 O      -0.178505     2.310095     0.715984     237.89
 C      -0.184736    -0.243905     0.333391      31.08
 H       0.819615    -0.439399     0.823315      16.98
 C      -2.228953    -1.205233    -0.422006      42.50
 C      -3.012881    -2.421126    -1.101423      77.57
 H      -3.885806    -1.971166    -1.493935      23.33
 O      -2.364705    -3.147878    -2.071390     287.95
 H      -2.842337    -3.923128    -2.307263      22.62
 C      -3.584934    -3.482775     0.080567      88.99
 H      -2.748067    -4.058346     0.263506      22.40
 O      -4.163719    -2.774060     1.191741     365.33
 H      -3.499014    -2.647794     2.044395      21.16
 C      -4.650171    -4.562132    -0.402047      99.92
 O      -4.025201    -5.445992    -1.289344     346.09
 H      -3.255558    -6.112027    -0.938976      27.02
 H      -5.457547    -4.158057    -0.883694      28.09
 H      -4.942645    -5.232914     0.472289      25.50
55
name = lig-etoh-frame_40
 C       2.847564     1.463333    -2.078468      31.40
 H       2.485923     2.333636    -2.638736      19.21
 C       3.440437     0.789782     0.173344      54.59
 H       3.157815     0.805817     1.190200      18.22
 C       3.895400    -0.501456    -0.382068       9.57
 O       4.228354    -1.316503     0.628909     228.57
 C       5.747227    -1.405130     0.862499      90.94
 H       5.700257    -2.389031     1.443029      24.37
 H       5.833046    -0.418519     1.411028      25.63
 H       6.255762    -1.353105    -0.115755      27.87
 C       3.980502    -0.882474    -1.799839       6.49
 O       4.435533    -2.055358    -2.240193     192.86
 H       4.489728    -2.806834    -1.385673      20.13
 C       3.397464     0.283633    -2.574994      67.24
 H       3.041149    -0.139551    -3.502781      21.42
 C       2.784988     1.701640    -0.685198      34.76
 C       2.127273     3.058625    -0.192204     103.07
 H       2.545187     3.733981    -0.938903      22.00
 O       2.530986     3.178273     1.238292     258.93
 H       3.578760     3.533278     1.276838      27.09
 C       0.597558     3.188836    -0.199039      67.90
 H       0.174783     3.012334    -1.263237      19.17
 C       0.147819     4.604518     0.167585     108.03
 O       0.878118     5.616958    -0.508479     276.97
 H       0.840995     5.414945    -1.505342      28.70
 H       0.154612     4.838832     1.315869      24.76
 H      -0.786569     4.712983    -0.296391      24.28
 C      -0.898639    -1.372169     0.009519      36.56
 H      -0.559936    -2.366831    -0.114860      13.37
 C      -2.879688     0.137619    -0.457944      46.61
 H      -3.901518     0.223662    -0.415197      21.24
 C      -2.079718     1.216835    -0.173899       2.57
 O      -2.802300     2.450397    -0.115833     223.48
 C      -4.072954     2.674375     0.695149     100.85
 H      -4.585712     1.852913     0.113403      21.93
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 H      -3.738154     2.641091     1.758404      24.51
 H      -4.432025     3.704843     0.459084      25.39
 C      -0.685837     1.119337     0.246800      18.14
 O      -0.151727     2.299330     0.785817     211.61
 C      -0.227007    -0.175104     0.286899      53.69
 H       0.771470    -0.454022     0.751289      17.67
 C      -2.230830    -1.229394    -0.524622      36.84
 C      -3.002984    -2.432563    -1.078411      73.20
 H      -3.995477    -2.101227    -1.621748      21.60
 O      -2.374374    -3.136608    -2.099426     244.83
 H      -2.839053    -4.041166    -2.380767      20.99
 C      -3.626798    -3.469712     0.104490      93.52
 H      -2.615893    -4.012475     0.486712      20.32
 O      -4.206627    -2.795048     1.178646     389.47
 H      -3.460941    -2.679627     1.753541      28.06
 C      -4.593746    -4.561592    -0.429231      88.66
 O      -3.974223    -5.508892    -1.282627     357.61
 H      -3.339658    -5.887462    -0.740842      35.23
 H      -5.628861    -3.915610    -0.681833      26.28
 H      -4.935778    -5.125343     0.423290      27.80
55
name = lig-etoh-frame_41
 C       2.910066     1.431442    -1.994427      74.62
 H       2.578634     2.272219    -2.613200      24.64
 C       3.407238     0.743080     0.084441      33.13
 H       3.490722     0.993652     1.229106      18.27
 C       3.888768    -0.524457    -0.389243      14.15
 O       4.189854    -1.345908     0.609233     214.88
 C       5.720985    -1.310402     0.891537     105.01
 H       5.836889    -2.217761     1.456818      27.01
 H       5.864068    -0.429562     1.449941      27.69
 H       6.457824    -1.572317     0.012310      26.29
 C       3.898794    -0.840615    -1.775627      28.27
 O       4.427428    -2.051526    -2.241757     264.45
 H       4.225149    -2.694919    -1.638361      30.10
 C       3.434605     0.277535    -2.541676      67.68
 H       2.788789    -0.217918    -3.435269      17.52
 C       2.828760     1.733541    -0.657399      24.03
 C       2.128046     3.051245    -0.172610     113.98
 H       2.474365     3.974542    -0.829522      19.67
 O       2.540259     3.158735     1.181169     324.79
 H       3.436696     3.349184     1.131734      31.44
 C       0.625653     3.185455    -0.181498      73.70
 H       0.235633     2.851659    -1.096395      21.06
 C       0.125914     4.543604     0.239516     107.16
 O       0.848733     5.625153    -0.564356     243.42
 H       0.635360     5.432350    -1.520358      28.39
 H      -0.074919     4.946852     1.231435      25.01
 H      -0.968386     4.620015    -0.121060      22.45
 C      -0.910627    -1.332947     0.021671      28.61
 H      -0.635051    -2.447458     0.178265      12.12
 C      -2.867187     0.143997    -0.446280      41.73
 H      -4.009814     0.519210    -0.450890      16.74
 C      -2.110668     1.170109    -0.226033      12.93
 O      -2.758114     2.518009    -0.091838     176.78
 C      -4.092343     2.613788     0.664629     104.52
 H      -4.883968     2.101291    -0.024010      21.48
 H      -3.643115     2.747472     1.671030      22.30
 H      -4.316146     3.766803     0.625142      24.61
 C      -0.755309     1.085426     0.242065       6.13
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 O      -0.094921     2.284586     0.838796     159.22
 C      -0.201925    -0.145084     0.279165      40.99
 H       0.948272    -0.222158     0.676630      15.34
 C      -2.254770    -1.227905    -0.625181      19.95
 C      -3.103844    -2.444102    -1.024307      83.83
 H      -3.969661    -2.049656    -1.480732      24.27
 O      -2.337624    -3.150686    -2.160536     241.97
 H      -2.860542    -3.975818    -2.199444      20.36
 C      -3.591287    -3.469313     0.097498     101.32
 H      -2.783096    -3.900729     0.610648      23.03
 O      -4.273285    -2.810614     1.162227     345.66
 H      -3.388710    -2.547188     1.709959      22.40
 C      -4.566661    -4.520502    -0.404607      94.61
 O      -3.929377    -5.567062    -1.310536     308.19
 H      -3.276492    -5.823279    -0.486443      26.08
 H      -5.388491    -4.070823    -0.831110      29.91
 H      -4.942398    -4.998450     0.555307      28.13
55
name = lig-etoh-frame_42
 C       2.955872     1.449979    -1.963836      80.37
 H       2.572466     2.048577    -2.816850      25.23
 C       3.380296     0.693859     0.077368      55.34
 H       3.803074     0.923395     1.002089      22.26
 C       3.853203    -0.477712    -0.408366      26.30
 O       4.216118    -1.423783     0.615370     230.86
 C       5.659786    -1.269934     0.915893     113.03
 H       5.985410    -2.046678     1.706729      26.31
 H       6.060128    -0.310627     1.493090      25.88
 H       6.291263    -1.487837     0.113326      28.33
 C       3.827121    -0.765148    -1.706808      35.87
 O       4.402109    -2.022929    -2.265336     234.91
 H       3.992194    -2.773289    -1.668277      26.77
 C       3.425291     0.186005    -2.566647      31.81
 H       3.015817     0.075340    -3.509888      13.43
 C       2.857743     1.783625    -0.656577      41.28
 C       2.172195     3.015743    -0.150655     123.62
 H       2.332890     4.023963    -0.605609      18.37
 O       2.537806     3.157434     1.148561     312.34
 H       3.598811     3.314319     1.218505      25.91
 C       0.622568     3.135989    -0.122382      62.80
 H       0.253004     2.801848    -1.179839      18.69
 C       0.055641     4.549094     0.237185      96.57
 O       0.812138     5.624927    -0.589758     212.84
 H       0.470750     5.505515    -1.638206      23.20
 H       0.092977     4.846990     1.318905      24.98
 H      -1.004497     4.413057     0.102709      23.97
 C      -0.995128    -1.319960    -0.029777      38.00
 H      -0.507982    -2.157863     0.419779      13.16
 C      -2.914064     0.032924    -0.493971      43.38
 H      -3.872019     0.297200    -0.707632      19.19
 C      -2.116401     1.271980    -0.207519       9.00
 O      -2.704378     2.573531    -0.079540     200.66
 C      -4.052083     2.618982     0.606137     107.41
 H      -5.079862     2.184858     0.357753      24.63
 H      -3.981122     2.251161     1.727400      24.87
 H      -4.258864     3.661433     0.498447      26.28
 C      -0.823325     1.135993     0.241285      -9.32
 O      -0.040698     2.233102     0.863296     186.03
 C      -0.115088    -0.162719     0.300412       9.28
 H       0.886672    -0.050098     0.608086      15.58
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 C      -2.272638    -1.191546    -0.650063      34.42
 C      -3.183989    -2.448491    -0.989550      63.02
 H      -4.157410    -1.943172    -1.385742      22.94
 O      -2.317844    -3.162810    -2.193839     188.25
 H      -2.777960    -4.021714    -2.158810      19.05
 C      -3.539026    -3.457329     0.074097      90.07
 H      -2.648831    -4.015697     0.585940      20.09
 O      -4.326753    -2.803426     1.158178     306.23
 H      -3.755607    -2.357206     1.818683      27.56
 C      -4.535668    -4.511783    -0.374617      79.91
 O      -3.882638    -5.599411    -1.292270     264.68
 H      -3.145274    -6.075613    -0.728333      26.84
 H      -5.357248    -4.141679    -1.213471      26.17
 H      -4.917338    -4.943409     0.542871      27.82
55
name = lig-etoh-frame_43
 C       2.985568     1.455383    -2.061979      55.63
 H       2.519298     2.009380    -2.867050      14.61
 C       3.366761     0.715840     0.141342      52.39
 H       3.897053     0.833213     1.157234      19.68
 C       3.816774    -0.461164    -0.346173       5.96
 O       4.280761    -1.490113     0.619617     233.60
 C       5.613906    -1.253734     0.991697     114.22
 H       5.906922    -1.859491     1.835576      26.89
 H       5.890448    -0.258094     1.236542      29.01
 H       6.154963    -1.356471    -0.084404      24.84
 C       3.807774    -0.801193    -1.717957      20.55
 O       4.349586    -1.968549    -2.265601     212.07
 H       3.845405    -2.831101    -1.794262      22.66
 C       3.358958     0.173643    -2.590932      73.83
 H       3.519663     0.260190    -3.828634      26.34
 C       2.879881     1.801833    -0.689447      59.46
 C       2.197222     3.001072    -0.130051     124.42
 H       2.436788     3.944812    -0.752649      21.91
 O       2.569970     3.171058     1.198043     349.19
 H       3.534737     3.384746     1.406066      29.81
 C       0.591807     3.056259    -0.083657      79.57
 H       0.309939     2.922690    -1.083722      21.43
 C       0.011860     4.571365     0.213428      98.97
 O       0.732923     5.607563    -0.596309     256.84
 H       0.592331     5.531994    -1.489468      31.39
 H       0.538553     4.639672     1.228657      24.60
 H      -1.104518     4.412691     0.122736      23.92
 C      -0.996943    -1.268615    -0.067896      50.97
 H      -0.525216    -2.177402     0.390797      13.13
 C      -2.921994     0.005394    -0.570233      37.80
 H      -4.027336    -0.069583    -1.090186      17.31
 C      -2.164756     1.353826    -0.163909       9.03
 O      -2.684965     2.598222    -0.071738     237.17
 C      -3.997530     2.631038     0.590787     108.97
 H      -4.979747     2.022901     0.355201      23.88
 H      -4.165586     1.968885     1.467564      24.71
 H      -4.240690     3.800504     0.530740      24.39
 C      -0.798296     1.181582     0.263560      -0.20
 O      -0.004286     2.160403     0.862296     226.73
 C      -0.157152    -0.162971     0.285332      19.83
 H       1.047615    -0.106352     0.708642      13.38
 C      -2.307719    -1.200566    -0.614983      29.07
 C      -3.202285    -2.411262    -1.008910      62.03
 H      -4.179312    -2.098271    -1.341762      25.21
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 O      -2.343375    -3.158910    -2.183891     171.89
 H      -2.598907    -4.193106    -2.257846      17.23
 C      -3.491875    -3.445288     0.095955      84.90
 H      -2.574454    -3.984023     0.366442      21.87
 O      -4.386828    -2.788357     1.145655     293.54
 H      -3.911999    -2.320940     1.842676      28.89
 C      -4.497859    -4.546309    -0.411171      89.81
 O      -3.831033    -5.620350    -1.251192     319.66
 H      -3.153498    -6.182609    -0.923630      32.00
 H      -5.157762    -4.220584    -1.177159      29.00
 H      -5.011332    -4.993161     0.458336      27.12
55
name = lig-etoh-frame_44
 C       2.975038     1.459955    -2.186319      61.31
 H       2.521349     2.258156    -2.824725      18.00
 C       3.383237     0.796062     0.246432      36.79
 H       3.504725     0.918386     1.321225      16.29
 C       3.792160    -0.522783    -0.273069     -17.25
 O       4.317349    -1.517128     0.612248     260.85
 C       5.614539    -1.224183     1.012648     103.98
 H       5.863678    -1.868725     1.895422      25.56
 H       5.569945    -0.036913     1.101546      24.96
 H       6.220944    -1.414066     0.188571      27.75
 C       3.793304    -0.854628    -1.749741       4.64
 O       4.281972    -1.938546    -2.257962     273.59
 H       3.934734    -2.667633    -1.956421      30.53
 C       3.316122     0.221979    -2.661688      77.18
 H       3.846498     0.103745    -3.517991      25.53
 C       2.906122     1.749292    -0.743224      28.06
 C       2.204288     3.023059    -0.113752     107.02
 H       2.572746     3.728787    -0.929199      22.35
 O       2.602808     3.197615     1.305700     320.84
 H       3.561726     3.500635     1.380688      29.36
 C       0.578205     3.020914    -0.083311      66.01
 H       0.232929     2.790488    -1.172689      18.47
 C       0.047801     4.549134     0.194121     103.95
 O       0.632832     5.588339    -0.554987     251.14
 H       0.708629     5.380484    -1.676010      23.74
 H       0.563037     4.670313     1.102621      25.53
 H      -1.045135     4.681744     0.199248      24.48
 C      -0.928679    -1.241068    -0.073537      52.08
 H      -0.693063    -2.309984     0.038691      18.26
 C      -2.946534     0.095411    -0.673235      27.41
 H      -3.805542    -0.099788    -1.192220      21.74
 C      -2.198334     1.322126    -0.124020      -0.43
 O      -2.707138     2.618248    -0.065378     219.08
 C      -3.982952     2.649333     0.581134      96.51
 H      -4.685399     2.051274    -0.325487      21.66
 H      -3.788673     2.119798     1.568869      23.78
 H      -4.251660     3.611311     0.814429      26.57
 C      -0.764955     1.165383     0.282465      17.10
 O       0.023352     2.097089     0.852563     240.08
 C      -0.248033    -0.121662     0.260967      39.37
 H       0.635234    -0.348594     0.649091      17.61
 C      -2.334207    -1.236311    -0.553549      42.23
 C      -3.153505    -2.404840    -1.050056      59.16
 H      -4.176081    -2.160008    -1.497446      22.28
 O      -2.394570    -3.145880    -2.150457     257.61
 H      -2.547544    -4.064051    -2.193998      21.65
 C      -3.495332    -3.433369     0.121245      88.46
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 H      -2.490895    -3.859769     0.445014      19.59
 O      -4.437381    -2.783622     1.114807     282.03
 H      -3.754399    -2.383613     1.820411      23.81
 C      -4.404720    -4.624520    -0.455167      80.79
 O      -3.794851    -5.622856    -1.228949     293.46
 H      -3.050818    -6.272286    -0.640920      24.01
 H      -5.228402    -4.093740    -1.182293      25.87
 H      -5.075494    -5.046322     0.336914      25.54
55
name = lig-etoh-frame_45
 C       2.921562     1.513015    -2.243685      48.15
 H       2.715655     2.429719    -2.798431      19.69
 C       3.406918     0.824722     0.288216      44.00
 H       3.025134     1.122051     1.341534      11.92
 C       3.762545    -0.577858    -0.243814      -5.76
 O       4.315702    -1.521447     0.586556     239.02
 C       5.637450    -1.149219     1.030372     105.37
 H       5.838573    -1.719577     1.970791      25.95
 H       5.567194    -0.143237     1.257577      26.82
 H       6.591913    -1.565658     0.385128      24.86
 C       3.718570    -0.779537    -1.694724       3.82
 O       4.248322    -1.942993    -2.288970     185.45
 H       3.897039    -2.882080    -1.865625      22.64
 C       3.338800     0.221422    -2.692823      43.46
 H       3.962877    -0.112187    -3.686313      19.75
 C       2.915125     1.665081    -0.761256      16.85
 C       2.211625     3.014906    -0.106605     106.89
 H       2.558971     3.839689    -0.772191      22.17
 O       2.625058     3.234497     1.396474     250.52
 H       3.624986     3.612403     1.249643      28.67
 C       0.583911     3.038909    -0.150060      67.02
 H       0.239728     2.590209    -1.044036      19.39
 C       0.111689     4.490107     0.198061     102.17
 O       0.548527     5.583338    -0.562378     310.78
 H       0.750502     5.249643    -1.422670      30.80
 H       0.365439     4.789557     1.314967      23.55
 H      -0.971034     4.719912     0.326750      23.14
 C      -0.970497    -1.297995    -0.116182      37.49
 H      -0.492459    -2.288152    -0.256525      18.25
 C      -2.893429     0.183203    -0.739179      32.12
 H      -3.959599     0.312972    -1.306124      22.04
 C      -2.204117     1.240755    -0.108712       3.56
 O      -2.703290     2.643368    -0.068527     209.59
 C      -3.990707     2.608946     0.554992     110.16
 H      -4.337117     2.446780    -0.402727      21.08
 H      -3.722236     2.213766     1.519231      22.49
 H      -4.390798     3.669192     1.002290      24.44
 C      -0.820549     1.123107     0.281344      25.49
 O       0.055788     2.064909     0.850943     210.47
 C      -0.332206    -0.105656     0.239210      21.72
 H       0.748468    -0.518114     0.789215      13.88
 C      -2.330108    -1.188904    -0.500771      24.62
 C      -3.100684    -2.444666    -1.085763      70.29
 H      -4.004756    -2.048867    -1.598818      21.41
 O      -2.436948    -3.106288    -2.110798     260.75
 H      -2.708017    -4.082259    -1.991079      18.50
 C      -3.534974    -3.436716     0.119628      96.30
 H      -2.615283    -3.629976     0.775692      19.93
 O      -4.440879    -2.783148     1.081583     339.40
 H      -3.763594    -2.527870     1.690209      27.52
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 C      -4.345106    -4.665456    -0.494798     101.35
 O      -3.720310    -5.658009    -1.210730     385.51
 H      -3.288152    -5.975855    -0.467050      31.16
 H      -5.068221    -4.080805    -1.041000      28.35
 H      -4.935014    -5.101530     0.311891      26.22
55
name = lig-etoh-frame_46
 C       2.890695     1.542370    -2.229087      66.26
 H       2.885807     2.426789    -2.867480      25.07
 C       3.399211     0.777396     0.252505      43.85
 H       2.838558     1.149309     1.107306      14.96
 C       3.718398    -0.547142    -0.240999      12.51
 O       4.320215    -1.531214     0.554786     229.62
 C       5.686901    -1.116188     1.068974     104.96
 H       5.720830    -1.538996     2.091513      26.04
 H       5.822167     0.012517     1.384761      24.99
 H       6.426791    -1.494468     0.491561      28.22
 C       3.636914    -0.693251    -1.615917       6.32
 O       4.212076    -1.968714    -2.321778     158.26
 H       3.951230    -2.777321    -1.678830      23.07
 C       3.413451     0.215231    -2.702233       3.56
 H       3.515240    -0.056107    -3.698284      17.63
 C       2.891693     1.633512    -0.749733      38.12
 C       2.217799     2.977292    -0.094796     103.96
 H       2.510134     4.060014    -0.420456      19.10
 O       2.637416     3.276846     1.421284     269.80
 H       3.542196     3.543430     1.409558      32.81
 C       0.624492     3.060494    -0.190177      58.69
 H       0.273411     2.617349    -1.180833      17.81
 C       0.130304     4.441928     0.271640     101.02
 O       0.493379     5.593724    -0.575810     295.31
 H       0.733083     5.258852    -1.542974      25.71
 H       0.339796     4.582190     1.271886      25.97
 H      -0.997449     4.300968     0.265061      22.42
 C      -1.063306    -1.365241    -0.183889      46.96
 H      -0.291057    -2.125908    -0.355680      15.66
 C      -2.845873     0.217952    -0.776596      58.07
 H      -3.718990     0.720630    -1.094613      23.48
 C      -2.197583     1.239256    -0.120366       9.53
 O      -2.635212     2.651995    -0.078166     200.47
 C      -3.995461     2.636799     0.559974      93.78
 H      -4.914992     2.397790    -0.308903      23.48
 H      -4.147977     1.792494     1.431517      22.96
 H      -4.284093     3.584083     0.795330      26.55
 C      -0.897835     1.110108     0.297429       0.01
 O       0.075319     2.056433     0.848493     170.11
 C      -0.311473    -0.220912     0.259359       8.52
 H       0.586368    -0.157055     0.640812      17.11
 C      -2.348623    -1.119518    -0.521547      34.45
 C      -3.084908    -2.432183    -1.062894      74.54
 H      -3.997218    -1.911450    -1.500476      20.56
 O      -2.447498    -3.101478    -2.089638     253.91
 H      -2.775544    -4.079157    -1.922084      14.51
 C      -3.564203    -3.433583     0.108809     101.42
 H      -2.754799    -3.647210     0.796728      20.64
 O      -4.436430    -2.784715     1.035093     333.57
 H      -3.842652    -2.507825     1.790112      26.89
 C      -4.333090    -4.639194    -0.480711      86.20
 O      -3.631496    -5.695686    -1.217507     318.12
 H      -3.057057    -6.156353    -0.349463      19.56
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 H      -5.118829    -4.124650    -1.203532      25.75
 H      -4.782257    -5.161423     0.426775      25.41
55
name = lig-etoh-frame_47
 C       2.922032     1.503569    -2.171926      88.54
 H       2.864543     2.339884    -2.894671      26.32
 C       3.328749     0.718016     0.165192      49.48
 H       3.058639     0.932514     1.234664      17.22
 C       3.694096    -0.481800    -0.229607      13.54
 O       4.344002    -1.525810     0.529161     216.16
 C       5.689215    -1.073632     1.157674      90.01
 H       5.623869    -1.534473     2.187570      24.63
 H       5.948391    -0.018224     1.118537      27.26
 H       6.411199    -1.542722     0.316798      24.12
 C       3.612126    -0.697133    -1.640090      18.39
 O       4.153245    -1.970919    -2.308263     206.03
 H       4.072413    -2.563457    -1.650359      28.67
 C       3.433309     0.283699    -2.637276      31.86
 H       3.116490    -0.019873    -3.743377      17.88
 C       2.847503     1.697399    -0.750738      35.71
 C       2.234302     2.969996    -0.056766     107.06
 H       2.543854     3.905785    -0.432068      20.06
 O       2.604244     3.291885     1.409378     259.19
 H       3.686047     3.452600     1.540486      27.04
 C       0.696945     3.043281    -0.191425      57.57
 H       0.396380     2.953682    -1.246950      19.49
 C       0.087631     4.383097     0.302792      90.25
 O       0.453060     5.592473    -0.575139     242.46
 H       0.531505     5.413000    -1.634540      24.92
 H       0.559809     4.459952     1.376690      22.94
 H      -0.920277     4.025222     0.165979      22.38
 C      -1.054291    -1.363127    -0.216438      48.06
 H      -0.498053    -2.318234    -0.397380      16.99
 C      -2.809093     0.236705    -0.762303      50.32
 H      -3.828124     0.647642    -1.117522      23.53
 C      -2.152590     1.335488    -0.141671      18.14
 O      -2.603868     2.623477    -0.075864     210.66
 C      -4.042117     2.621943     0.518612     105.58
 H      -4.961406     2.355529     0.187737      26.23
 H      -4.360162     1.790386     1.086279      24.86
 H      -4.098751     3.783097     0.814860      23.96
 C      -0.879202     1.053346     0.347721       8.11
 O       0.066805     2.053332     0.824393     138.65
 C      -0.331768    -0.303039     0.277392       6.12
 H       0.866248    -0.024309     0.544369      12.86
 C      -2.418575    -1.105751    -0.628485      42.64
 C      -3.135703    -2.346144    -0.996575      85.13
 H      -4.152558    -1.990512    -1.329618      21.52
 O      -2.435676    -3.131429    -2.084497     254.09
 H      -2.640544    -4.040556    -2.080165      18.33
 C      -3.560500    -3.405099     0.087166      86.85
 H      -2.612390    -3.966022     0.557065      18.33
 O      -4.450129    -2.771021     0.997520     307.79
 H      -3.979876    -2.465563     1.864266      25.21
 C      -4.351677    -4.611360    -0.450723      92.54
 O      -3.531563    -5.721557    -1.204889     328.74
 H      -2.830895    -6.238812    -0.800635      29.84
 H      -5.126919    -4.473692    -1.242194      26.67
 H      -4.775049    -5.070354     0.400071      27.13
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name = lig-etoh-frame_48
 C       2.974587     1.500915    -2.085206      73.04
 H       2.647947     2.229954    -2.810453      24.17
 C       3.194017     0.736205     0.137800      60.38
 H       3.548649     0.707237     1.234294      19.50
 C       3.726241    -0.507252    -0.282745       6.17
 O       4.369328    -1.481762     0.514872     249.52
 C       5.671798    -1.071707     1.190302     104.41
 H       5.720987    -1.492931     2.163492      26.73
 H       5.829096     0.020473     0.959099      27.68
 H       6.353270    -1.619006     0.583770      26.72
 C       3.655356    -0.775838    -1.734534      15.01
 O       4.069272    -1.930250    -2.272899     156.33
 H       4.277624    -2.631143    -1.399266      20.93
 C       3.388581     0.331366    -2.571256      66.35
 H       3.070159     0.053741    -3.543706      20.52
 C       2.808416     1.791596    -0.729356      43.94
 C       2.263839     2.985229    -0.004629     103.33
 H       2.672244     3.789661    -0.834613      20.33
 O       2.571074     3.281386     1.384375     334.62
 H       3.527625     3.338225     1.418578      28.78
 C       0.769574     3.027749    -0.162031      62.48
 H       0.525256     3.043032    -1.245859      18.83
 C       0.075547     4.321439     0.293585      93.17
 O       0.406295     5.577869    -0.551496     252.92
 H       0.343287     5.395440    -1.460183      30.94
 H       0.511429     4.589588     1.227524      24.79
 H      -1.059832     4.160287     0.290711      22.06
 C      -1.028424    -1.356594    -0.245016      21.98
 H      -0.912899    -2.445325    -0.335593      16.42
 C      -2.836374     0.276314    -0.729300      33.81
 H      -3.853412     0.175237    -1.195859      20.62
 C      -2.065054     1.394443    -0.170354      12.60
 O      -2.641265     2.592044    -0.072797     183.42
 C      -4.065954     2.653040     0.490238      80.42
 H      -4.981495     2.516541    -0.312945      22.45
 H      -3.964426     1.832056     1.402909      22.65
 H      -3.971930     3.543646     1.051944      25.02
 C      -0.798072     0.992480     0.397490      14.59
 O       0.046231     2.042280     0.778303     176.90
 C      -0.305999    -0.292382     0.305733      48.41
 H       0.700353    -0.507186     0.353593      17.67
 C      -2.422931    -1.107138    -0.735311      23.01
 C      -3.246165    -2.304298    -0.968618      83.35
 H      -4.278825    -2.126254    -1.344606      23.51
 O      -2.413844    -3.128792    -2.082759     171.80
 H      -2.657979    -4.167775    -2.115329      14.29
 C      -3.517060    -3.389178     0.062651      95.68
 H      -2.673669    -3.929217     0.348734      21.79
 O      -4.474926    -2.747824     0.985253     306.76
 H      -3.972787    -2.508177     1.742960      29.57
 C      -4.339875    -4.648885    -0.448758      76.63
 O      -3.469715    -5.703811    -1.232127     294.93
 H      -2.655191    -6.120523    -0.727555      26.86
 H      -5.154723    -4.598984    -1.215679      26.65
 H      -4.875408    -5.066014     0.491880      26.56
55
name = lig-etoh-frame_49
 C       2.984587     1.593293    -1.993592      35.62
 H       2.438301     2.220160    -2.737247      20.13
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 C       3.122815     0.711454     0.163959      54.30
 H       3.610099     0.891961     1.087030      23.03
 C       3.761651    -0.537049    -0.406426      10.91
 O       4.387036    -1.427577     0.513192     244.91
 C       5.630822    -1.082581     1.168836      97.86
 H       5.739949    -1.303608     2.312545      25.00
 H       5.713478     0.047414     1.052507      26.77
 H       6.542836    -1.741449     0.765308      24.43
 C       3.718624    -0.807734    -1.766395      19.93
 O       3.993659    -1.948570    -2.228057     231.25
 H       4.464998    -2.439158    -1.532864      23.17
 C       3.328136     0.291833    -2.523394      63.40
 H       3.211385     0.140552    -3.653789      23.45
 C       2.799434     1.823664    -0.633553      62.30
 C       2.293089     3.051145    -0.010689     114.83
 H       2.578187     3.746775    -0.731072      25.97
 O       2.537025     3.255660     1.338817     340.22
 H       3.575252     3.364870     1.396646      25.77
 C       0.781310     3.030617    -0.134570      53.76
 H       0.597374     2.742130    -1.218457      20.11
 C       0.064757     4.318008     0.260853     104.47
 O       0.356842     5.545105    -0.492822     228.98
 H       0.190343     5.268313    -1.556155      25.17
 H       0.370629     4.734271     1.277967      23.89
 H      -0.979052     4.336708     0.444689      24.30
 C      -1.094163    -1.353247    -0.289568      32.35
 H      -0.905904    -2.454504    -0.127014      17.11
 C      -2.877523     0.262775    -0.703522      35.08
 H      -3.869004     0.234325    -1.143218      20.01
 C      -2.013961     1.333285    -0.211082      -0.90
 O      -2.697244     2.600480    -0.073268     204.88
 C      -4.051621     2.635049     0.491227     109.10
 H      -4.417719     2.765776    -0.497106      21.49
 H      -3.870781     2.057454     1.295043      24.10
 H      -4.091699     3.587261     1.186189      24.53
 C      -0.720807     1.005557     0.397363      13.86
 O       0.049972     2.034576     0.740382     213.42
 C      -0.267107    -0.335522     0.302399      40.26
 H       0.804095    -0.846735     0.439895      16.82
 C      -2.342732    -1.066143    -0.780513      20.48
 C      -3.348544    -2.327885    -1.022314      68.44
 H      -4.347090    -2.102980    -1.542351      22.81
 O      -2.400244    -3.116653    -2.081704     201.89
 H      -2.783666    -4.005497    -1.993693      18.13
 C      -3.531923    -3.383770     0.023596      79.25
 H      -2.473238    -3.713798     0.562196      18.76
 O      -4.487269    -2.734268     0.984925     291.66
 H      -3.838705    -2.488516     1.733020      25.22
 C      -4.307149    -4.733392    -0.463853      84.24
 O      -3.422025    -5.657893    -1.258330     363.03
 H      -2.865185    -5.851861    -0.433688      26.84
 H      -5.183554    -4.423785    -1.180557      26.93
 H      -4.716850    -5.125659     0.430375      28.67
55
name = lig-etoh-frame_50
 C       2.951461     1.660053    -1.948661      33.06
 H       2.505165     2.361520    -2.637132      19.55
 C       3.153094     0.628302     0.183775      39.07
 H       3.362072     1.101203     1.244907      17.76
 C       3.775672    -0.483937    -0.438110      15.66
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 O       4.393608    -1.398479     0.507091     258.43
 C       5.610619    -1.082040     1.154358     123.54
 H       5.433742    -1.112378     2.207915      27.16
 H       5.834396    -0.021358     1.106256      28.24
 H       6.522264    -1.608508     0.885559      27.36
 C       3.749197    -0.740773    -1.745269      23.14
 O       3.953659    -2.055974    -2.236700     233.53
 H       4.579345    -2.451115    -1.598965      24.40
 C       3.245129     0.285431    -2.522109      65.77
 H       3.471308     0.296077    -3.625511      27.30
 C       2.821720     1.784250    -0.529413      44.58
 C       2.274221     3.110021    -0.036964      99.47
 H       2.553729     4.185485    -0.575845      21.43
 O       2.541834     3.235536     1.314518     318.50
 H       3.518694     3.528007     1.534202      28.33
 C       0.720194     3.022249    -0.139986      71.45
 H       0.530151     2.551354    -1.085973      21.88
 C       0.059299     4.385488     0.271147     103.68
 O       0.307630     5.499674    -0.470322     322.29
 H       0.232202     5.369004    -1.408689      30.05
 H       0.376154     4.573781     1.336090      24.85
 H      -1.094487     4.168248     0.376162      22.38
 C      -1.136273    -1.358051    -0.289644      46.75
 H      -0.695750    -2.291689    -0.051461      16.74
 C      -2.878765     0.222167    -0.688995      50.56
 H      -3.917351     0.697041    -0.971146      18.19
 C      -2.048764     1.238525    -0.236740     -12.11
 O      -2.677610     2.616690    -0.078724     194.98
 C      -3.971299     2.670051     0.505393      98.34
 H      -4.624750     2.752043    -0.464876      23.55
 H      -4.346132     1.622407     1.238195      22.34
 H      -4.287778     3.646120     0.912537      24.94
 C      -0.667978     1.018976     0.317874      -3.40
 O       0.099326     2.052121     0.743584     210.19
 C      -0.222088    -0.428837     0.260531      41.77
 H       0.731587    -0.703872     0.800293      18.35
 C      -2.346774    -1.039209    -0.801596      32.73
 C      -3.356328    -2.351147    -1.157608      68.22
 H      -4.259614    -2.009160    -1.653083      23.89
 O      -2.417083    -3.088243    -2.070746     246.23
 H      -2.775282    -3.987674    -2.033457      20.00
 C      -3.570674    -3.389571     0.020159      89.83
 H      -2.714159    -3.376910     0.576726      23.81
 O      -4.476014    -2.732652     0.997599     323.45
 H      -3.814214    -2.410387     1.708927      25.86
 C      -4.267317    -4.770963    -0.510551      90.60
 O      -3.392867    -5.584830    -1.248497     393.01
 H      -2.894529    -5.986803    -0.477728      24.60
 H      -5.088061    -4.342187    -1.050448      27.67
 H      -4.570703    -5.371853     0.439597      26.46
55
name = lig-etoh-frame_51
 C       2.901931     1.639329    -1.926821      63.48
 H       2.757273     2.580431    -2.529279      20.01
 C       3.227429     0.617470     0.252651      46.44
 H       3.041962     0.713249     1.292594      20.88
 C       3.805865    -0.419576    -0.324036      19.70
 O       4.385010    -1.394966     0.471482     244.00
 C       5.587023    -1.031348     1.171449      97.82
 H       5.150681    -1.151136     2.238384      23.12
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 H       6.042616     0.041343     0.946079      25.32
 H       6.472277    -1.701092     0.858632      25.10
 C       3.748790    -0.706948    -1.769711       7.54
 O       3.922191    -2.150597    -2.256952     142.73
 H       4.751205    -2.568748    -1.608354      21.44
 C       3.181672     0.379393    -2.549308      67.60
 H       3.476279     0.330420    -3.577562      26.72
 C       2.850223     1.747848    -0.527337      22.60
 C       2.237999     3.167960    -0.058997     101.29
 H       2.503570     4.056993    -0.450676      23.34
 O       2.558635     3.232811     1.350605     319.86
 H       3.432984     3.606294     1.441983      29.54
 C       0.642209     3.025384    -0.160572      67.61
 H       0.337733     2.669786    -1.226212      19.73
 C      -0.001694     4.390591     0.319350     108.03
 O       0.279316     5.505055    -0.463909     337.31
 H       0.321871     5.384972    -1.465992      28.08
 H       0.447245     4.439931     1.322203      25.69
 H      -0.978715     4.040641     0.222835      24.19
 C      -1.093265    -1.365629    -0.243444      52.19
 H      -0.674543    -2.453713    -0.219066      16.66
 C      -2.897419     0.234878    -0.687954      63.46
 H      -3.790802     0.697521    -0.835131      22.96
 C      -2.060241     1.205682    -0.208621       2.55
 O      -2.605068     2.603206    -0.074951     214.58
 C      -3.965398     2.660669     0.483109     130.69
 H      -4.926087     2.522941    -0.131938      25.45
 H      -4.500753     1.864692     0.820836      26.19
 H      -4.164537     3.673685     0.883080      26.43
 C      -0.653522     0.980515     0.180903       6.39
 O       0.163609     2.060399     0.788674     194.24
 C      -0.214739    -0.419373     0.230194      47.76
 H       0.620055    -0.560819     0.957117      18.00
 C      -2.463366    -1.098514    -0.826717      27.17
 C      -3.272374    -2.359536    -1.290448      74.27
 H      -4.248576    -1.917040    -1.779567      22.53
 O      -2.452350    -3.059491    -2.070957     247.93
 H      -2.610946    -4.099756    -2.208124      15.90
 C      -3.652750    -3.355152     0.013793      64.29
 H      -2.551967    -3.383224     0.551485      19.03
 O      -4.468519    -2.733737     1.014671     340.32
 H      -3.900072    -2.371095     1.661723      30.66
 C      -4.218670    -4.758971    -0.485713      95.40
 O      -3.359292    -5.515746    -1.254104     353.79
 H      -2.779139    -6.261243    -0.785050      23.03
 H      -5.223687    -4.441358    -1.094842      25.38
 H      -4.547017    -5.410054     0.286375      26.11
55
name = lig-etoh-frame_52
 C       2.861333     1.604043    -1.921115      48.03
 H       3.008879     2.569940    -2.400476      22.58
 C       3.264773     0.715123     0.356094      39.73
 H       2.877813     0.270081     1.388453      20.07
 C       3.857380    -0.437783    -0.274384      -0.97
 O       4.383111    -1.412565     0.423521     218.59
 C       5.574569    -0.968533     1.207940     109.34
 H       5.363141    -1.120112     2.228181      26.78
 H       5.941759    -0.070490     0.870953      28.27
 H       6.184888    -1.892418     0.986075      25.18
 C       3.713929    -0.690985    -1.775647       2.18
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 O       3.909467    -2.185375    -2.256710     193.47
 H       4.586340    -2.535097    -1.785602      27.51
 C       3.177996     0.451342    -2.573329      47.42
 H       3.231507     0.344288    -3.749692      20.34
 C       2.859022     1.760667    -0.566591      27.82
 C       2.182693     3.119174    -0.032711      99.62
 H       2.627138     4.057258    -0.735932      20.78
 O       2.554761     3.242051     1.406752     265.11
 H       3.555419     3.654789     1.301110      24.85
 C       0.594535     3.058455    -0.195402      77.62
 H       0.249423     2.988636    -1.193537      20.12
 C      -0.059249     4.322977     0.342475      84.50
 O       0.261341     5.556361    -0.465439     248.18
 H       0.502747     5.244055    -1.495078      25.40
 H       0.388265     4.528012     1.399238      22.61
 H      -1.217435     4.141010     0.310720      20.88
 C      -1.079896    -1.417037    -0.232841      28.35
 H      -0.872375    -2.417145    -0.398460      16.95
 C      -2.915251     0.226525    -0.691693      32.26
 H      -4.075487     0.461599    -0.943404      23.82
 C      -2.010127     1.248232    -0.150520       6.52
 O      -2.540162     2.548842    -0.066004     155.11
 C      -4.000152     2.673696     0.408458      80.87
 H      -4.778688     2.692908    -0.382400      25.11
 H      -4.264516     1.651919     1.264298      22.67
 H      -3.860956     3.598073     1.106811      23.36
 C      -0.662988     0.955860     0.064167      19.45
 O       0.201773     2.018135     0.822125     143.16
 C      -0.239908    -0.325646     0.211990      34.71
 H       0.655872    -0.557510     0.981055      16.69
 C      -2.526881    -1.181154    -0.808961      11.48
 C      -3.245961    -2.327420    -1.340337      96.95
 H      -4.135630    -2.026586    -1.867648      23.08
 O      -2.436858    -3.073833    -2.142123     272.72
 H      -2.626399    -3.999446    -2.140250      19.03
 C      -3.672041    -3.297804     0.009998      90.71
 H      -2.732511    -3.654165     0.260701      23.63
 O      -4.487979    -2.737794     1.020119     327.72
 H      -3.814670    -2.329412     1.714262      24.76
 C      -4.217856    -4.706548    -0.433911     104.12
 O      -3.311540    -5.451839    -1.336790     359.97
 H      -2.864321    -6.159557    -0.788557      25.83
 H      -5.081857    -4.685017    -1.081531      26.18
 H      -4.629290    -5.334969     0.434698      26.38
55
name = lig-etoh-frame_53
 C       2.858469     1.611051    -1.932273      60.30
 H       2.951152     2.527199    -2.526626      24.58
 C       3.288583     0.783197     0.420178      37.30
 H       2.893114     0.406851     1.311343      21.49
 C       3.855080    -0.425906    -0.342977     -12.14
 O       4.406367    -1.455935     0.407186     198.49
 C       5.548621    -0.990907     1.240842      89.34
 H       5.532675    -0.846033     2.408412      24.89
 H       5.940733     0.061471     0.766410      24.39
 H       6.179260    -1.868428     1.114242      25.49
 C       3.663980    -0.684801    -1.748873       1.20
 O       3.870978    -2.135747    -2.262651     169.47
 H       4.660343    -2.543392    -1.709624      24.17
 C       3.226083     0.407115    -2.618356      34.09
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 H       2.958898     0.394649    -3.609939      20.84
 C       2.831384     1.792533    -0.512714      23.93
 C       2.152184     3.046385    -0.020645     126.99
 H       2.524267     3.699479    -0.676479      25.68
 O       2.552402     3.276558     1.427006     311.61
 H       3.483278     3.488207     1.430925      30.88
 C       0.590429     3.109514    -0.167091      63.26
 H       0.226916     3.027401    -1.283467      19.43
 C      -0.126685     4.298732     0.363278     104.33
 O       0.249945     5.586788    -0.475434     268.63
 H       0.556767     5.318425    -1.268153      32.91
 H       0.155664     4.593446     1.326244      25.52
 H      -1.152918     4.348513     0.508956      25.16
 C      -1.139268    -1.430027    -0.266530      47.50
 H      -0.776149    -2.542299    -0.384343      18.10
 C      -2.944627     0.172797    -0.694277      44.90
 H      -3.914338     0.234962    -0.997129      25.37
 C      -2.025315     1.274551    -0.144378       5.87
 O      -2.499849     2.491901    -0.049029     182.57
 C      -3.985912     2.648916     0.394794     102.80
 H      -4.401446     2.973535    -0.631430      22.78
 H      -3.921919     1.938705     1.222181      24.00
 H      -3.831587     3.419298     1.072707      26.43
 C      -0.655663     1.015141     0.033256      20.88
 O       0.200923     1.940434     0.792628     154.41
 C      -0.277827    -0.324757     0.196106      30.95
 H       0.608486    -0.485084     0.662464      20.08
 C      -2.467338    -1.166092    -0.731218      16.88
 C      -3.287325    -2.309925    -1.314497      76.03
 H      -4.228660    -2.087698    -1.981482      21.41
 O      -2.378772    -3.102408    -2.255507     188.16
 H      -2.732348    -4.089040    -1.998141      11.32
 C      -3.680167    -3.269488    -0.047056      75.36
 H      -2.634239    -3.781558     0.292332      15.23
 O      -4.495935    -2.729815     1.031631     314.66
 H      -3.804983    -2.402015     1.665099      25.35
 C      -4.264524    -4.654981    -0.399107      78.53
 O      -3.274205    -5.380151    -1.430486     304.17
 H      -2.830613    -5.909508    -0.648420      23.18
 H      -5.188482    -4.756999    -1.147950      24.95
 H      -4.436007    -5.140007     0.577060      27.93
55
name = lig-etoh-frame_54
 C       2.903670     1.623038    -1.943551      61.20
 H       2.590176     2.429825    -2.678449      23.00
 C       3.325233     0.786833     0.357451      44.23
 H       2.976866     0.819412     1.496914      18.88
 C       3.810809    -0.374921    -0.402760       3.02
 O       4.436431    -1.495043     0.413579     214.80
 C       5.541112    -1.009150     1.267641     115.80
 H       5.339819    -0.576372     2.228053      27.23
 H       5.940270    -0.205078     0.815822      29.23
 H       6.452954    -1.740994     1.240665      26.04
 C       3.618733    -0.714725    -1.738814      15.38
 O       3.830693    -2.021763    -2.256414     173.97
 H       4.612346    -2.465134    -1.613114      22.14
 C       3.271096     0.343230    -2.594152      64.10
 H       2.819531     0.263515    -3.690320      19.26
 C       2.789521     1.783837    -0.432621      34.70
 C       2.128356     2.981230     0.030388     104.80
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 H       2.571103     3.890598    -0.716350      21.38
 O       2.518607     3.313913     1.417517     268.38
 H       3.564771     3.403138     1.537014      26.83
 C       0.592265     3.118965    -0.108206      65.69
 H       0.391604     2.831120    -1.092923      21.45
 C      -0.162981     4.373230     0.377660      89.59
 O       0.224484     5.597084    -0.447965     207.76
 H       0.672415     5.351028    -1.425504      24.86
 H       0.208377     4.644565     1.493532      22.84
 H      -1.335012     4.304943     0.422310      22.04
 C      -1.164586    -1.430659    -0.296782      67.86
 H      -0.678602    -2.329193    -0.217131      22.22
 C      -2.905379     0.124492    -0.666004      66.92
 H      -3.999864     0.310494    -1.063912      22.86
 C      -2.098080     1.210854    -0.206425       3.17
 O      -2.482397     2.491094    -0.020653     194.81
 C      -3.872147     2.661331     0.360680      92.08
 H      -4.387985     2.937088    -0.542303      25.37
 H      -4.164164     1.607139     1.127496      22.00
 H      -3.957227     3.718934     0.987735      23.47
 C      -0.651997     1.064278     0.081356      13.92
 O       0.172393     1.869555     0.706462     169.63
 C      -0.359903    -0.385652     0.139879      20.43
 H       0.889138    -0.526948     0.329881      18.86
 C      -2.392392    -1.120829    -0.664947      35.23
 C      -3.324439    -2.324764    -1.281561      66.01
 H      -4.166711    -2.008344    -1.815510      23.43
 O      -2.351174    -3.131006    -2.341518     166.58
 H      -2.554496    -4.068901    -2.043857      11.92
 C      -3.658946    -3.288047    -0.124673      98.97
 H      -2.768202    -3.416257     0.401730      19.77
 O      -4.483916    -2.715842     1.028715     312.34
 H      -3.811591    -2.437850     1.685794      26.81
 C      -4.338799    -4.605305    -0.437180      89.93
 O      -3.257281    -5.315637    -1.465794     315.65
 H      -2.576534    -5.682016    -0.776141      23.76
 H      -5.274945    -4.600236    -0.879478      26.79
 H      -4.225996    -5.130122     0.549529      28.69
55
name = lig-etoh-frame_55
 C       2.947283     1.601975    -1.942153      47.62
 H       2.336751     2.249630    -2.514300      20.28
 C       3.343878     0.746948     0.278097      61.84
 H       3.478942     1.142998     1.284657      19.90
 C       3.783732    -0.365385    -0.361028       9.27
 O       4.461819    -1.513140     0.416449     227.99
 C       5.553083    -1.027652     1.269725     102.72
 H       4.969526    -0.558017     2.157258      24.08
 H       6.117710    -0.135733     0.625924      25.53
 H       6.361653    -1.673425     1.480427      27.19
 C       3.584828    -0.746450    -1.744662      15.05
 O       3.808314    -1.898297    -2.233392     238.96
 H       4.312616    -2.319314    -1.655033      28.10
 C       3.253424     0.345396    -2.551124      85.21
 H       3.072044     0.037138    -3.527515      24.54
 C       2.764955     1.745626    -0.473713      66.15
 C       2.135621     3.037401     0.092783     117.56
 H       2.424562     3.816227    -0.450949      26.71
 O       2.473241     3.347157     1.409955     329.94
 H       3.502898     3.424595     1.444115      28.01
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 C       0.594874     3.076677    -0.022074      61.88
 H       0.449642     2.733304    -1.127845      20.55
 C      -0.175001     4.491143     0.401120     115.95
 O       0.203421     5.591663    -0.421073     294.92
 H       0.544250     5.380001    -1.343826      28.23
 H       0.183332     4.611585     1.332184      27.07
 H      -1.151557     4.164243     0.197562      24.39
 C      -1.101128    -1.422828    -0.285693      50.23
 H      -0.649664    -2.468529    -0.172539      21.02
 C      -2.897436     0.147042    -0.640029      81.06
 H      -3.860614     0.420150    -0.992673      23.08
 C      -2.107528     1.145392    -0.269946      17.79
 O      -2.487240     2.520855     0.012794     229.28
 C      -3.765417     2.701740     0.359959     124.23
 H      -4.641373     2.669920    -0.537350      24.26
 H      -4.416806     1.703834     0.770881      23.30
 H      -3.968030     3.577162     0.796179      28.08
 C      -0.743609     0.960838     0.127778      22.29
 O       0.153923     1.850386     0.627283     187.58
 C      -0.340646    -0.378815     0.069738      52.66
 H       0.582742    -0.650279     0.070534      23.47
 C      -2.431797    -1.170803    -0.675833      35.19
 C      -3.282972    -2.338718    -1.251948      58.30
 H      -4.222556    -1.801346    -1.754501      21.56
 O      -2.365980    -3.119146    -2.380659     150.43
 H      -2.442641    -4.118850    -2.201498      12.82
 C      -3.651090    -3.286601    -0.165564      94.09
 H      -2.655001    -3.293650     0.445220      18.88
 O      -4.474987    -2.694135     0.998461     270.60
 H      -3.761445    -2.456618     1.739894      24.15
 C      -4.327702    -4.579739    -0.487707      75.55
 O      -3.268120    -5.252884    -1.464130     338.90
 H      -2.554228    -5.603429    -0.978886      28.89
 H      -5.520551    -4.440288    -0.706371      24.01
 H      -4.207467    -5.318042     0.357068      27.03
55
name = lig-etoh-frame_56
 C       2.934267     1.567782    -1.909522      60.96
 H       2.317675     2.374508    -2.439315      17.18
 C       3.367542     0.749365     0.233458      77.61
 H       3.963400     1.060648     1.159484      22.55
 C       3.799203    -0.466737    -0.289995      16.86
 O       4.487158    -1.515991     0.396742     261.83
 C       5.547933    -0.976581     1.244681     118.58
 H       4.953165    -0.626058     2.058565      25.23
 H       6.110160    -0.287377     0.773748      30.15
 H       6.110987    -1.885840     1.792769      25.28
 C       3.551011    -0.656136    -1.675243      18.83
 O       3.796975    -1.843964    -2.251407     153.41
 H       4.204084    -2.516414    -1.448319      20.47
 C       3.217921     0.363253    -2.496161      83.82
 H       3.331407     0.040401    -3.612862      23.25
 C       2.757375     1.731019    -0.604013      93.53
 C       2.127388     3.093122     0.140581     108.16
 H       2.455163     4.066593    -0.587134      24.01
 O       2.439206     3.372097     1.438315     319.77
 H       3.400001     3.616736     1.429977      28.17
 C       0.594785     3.015159     0.003807      80.39
 H       0.412183     3.048337    -1.060075      22.23
 C      -0.148068     4.529128     0.371400      97.50
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 O       0.189845     5.608324    -0.395051     298.45
 H       0.375922     5.318071    -1.291068      30.80
 H       0.075113     4.751731     1.559735      23.57
 H      -1.210099     4.176169     0.168705      22.83
 C      -1.081479    -1.465114    -0.279138      23.64
 H      -0.763031    -2.490231    -0.332761      17.08
 C      -2.936315     0.139163    -0.644452      41.11
 H      -3.969807     0.450475    -0.974671      20.00
 C      -2.047994     1.189662    -0.275187      23.72
 O      -2.462251     2.522723     0.026746     221.02
 C      -3.789650     2.714803     0.306860     117.35
 H      -4.398711     2.647823    -0.572053      26.15
 H      -4.434385     1.845865     0.879144      24.18
 H      -3.967395     3.726881     0.933578      24.52
 C      -0.851414     0.829405     0.155815      29.60
 O       0.131179     1.844645     0.589021     189.90
 C      -0.270836    -0.349384     0.001140      49.81
 H       0.924202    -0.711080     0.088732      17.14
 C      -2.480923    -1.263647    -0.714031      18.71
 C      -3.229064    -2.324287    -1.279169      95.94
 H      -4.057596    -1.907175    -1.723091      25.70
 O      -2.419458    -3.057151    -2.372971     182.29
 H      -2.595130    -4.118024    -2.312170      14.41
 C      -3.624260    -3.266308    -0.109038      98.90
 H      -2.665910    -3.636536     0.219776      22.59
 O      -4.461456    -2.664521     0.952114     337.06
 H      -3.821535    -2.491079     1.624762      29.21
 C      -4.268979    -4.596428    -0.525507     104.59
 O      -3.325343    -5.194259    -1.479815     342.51
 H      -2.649791    -5.707258    -0.840249      25.21
 H      -5.225138    -4.449343    -0.849644      28.05
 H      -4.369731    -5.345372     0.245438      30.00
55
name = lig-etoh-frame_57
 C       2.834358     1.601578    -1.954293      56.67
 H       2.641093     2.453677    -2.564097      16.76
 C       3.428715     0.764780     0.232038      76.91
 H       4.093088     0.976755     1.091006      21.86
 C       3.801788    -0.562774    -0.230530      22.24
 O       4.520762    -1.514853     0.359247     248.79
 C       5.512150    -0.984633     1.272577     115.73
 H       5.058276    -0.384123     2.163826      24.27
 H       6.352772    -0.223084     0.795557      26.22
 H       5.812069    -1.857860     1.718073      27.48
 C       3.540163    -0.596890    -1.574912      27.15
 O       3.809208    -1.852623    -2.268121     193.05
 H       3.940467    -2.542578    -1.534151      24.29
 C       3.192444     0.368440    -2.498531      38.25
 H       3.470250     0.357350    -3.542175      25.95
 C       2.773869     1.759709    -0.600395      50.24
 C       2.117561     3.146104     0.087762     112.73
 H       2.375046     3.906132    -0.503316      24.77
 O       2.422382     3.388737     1.493024     295.94
 H       3.377749     3.881750     1.573270      25.64
 C       0.588202     3.023783    -0.023792      66.12
 H       0.335747     3.226150    -1.127137      19.07
 C      -0.140400     4.468343     0.408044     104.55
 O       0.200804     5.653010    -0.385270     219.97
 H       0.203126     5.306854    -1.443256      25.54
 H      -0.150639     4.845051     1.346019      26.35
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 H      -1.218071     4.388389     0.329181      24.38
 C      -1.122167    -1.505216    -0.307107      44.83
 H      -0.705743    -2.518310    -0.486023      17.91
 C      -2.977560     0.099120    -0.673425      38.54
 H      -4.056305     0.330698    -0.940417      20.77
 C      -2.090698     1.244762    -0.262804       9.58
 O      -2.409562     2.503491     0.032414     172.56
 C      -3.877442     2.755604     0.265185      74.24
 H      -4.243962     2.939100    -0.860023      22.35
 H      -4.291966     1.781499     1.263664      20.51
 H      -3.881900     3.602809     0.842300      25.94
 C      -0.820543     0.817490     0.188155       2.80
 O       0.089946     1.816496     0.591678     199.92
 C      -0.148769    -0.457866    -0.063662      38.08
 H       0.830011    -0.337127     0.230879      19.72
 C      -2.442356    -1.240287    -0.719120      22.04
 C      -3.200410    -2.363635    -1.333699      77.77
 H      -4.217120    -2.013251    -1.871445      22.88
 O      -2.496300    -2.979747    -2.338253     262.43
 H      -2.823854    -3.833954    -2.274287      22.62
 C      -3.598033    -3.286711    -0.037227      81.16
 H      -2.631248    -3.833714     0.266854      20.46
 O      -4.434828    -2.638425     0.887925     335.62
 H      -3.808264    -2.401434     1.673224      25.86
 C      -4.203844    -4.610280    -0.555201      80.09
 O      -3.376448    -5.177337    -1.491565     341.55
 H      -2.932582    -5.803572    -0.878456      25.87
 H      -5.151943    -4.452946    -1.340629      24.62
 H      -4.561728    -5.271001     0.351415      26.52
55
name = lig-etoh-frame_58
 C       2.718010     1.660408    -2.031514      87.40
 H       2.911088     2.518146    -2.749463      22.61
 C       3.513225     0.768220     0.250838      51.35
 H       3.852094     1.168853     1.228736      19.40
 C       3.748361    -0.531438    -0.200995      26.49
 O       4.573677    -1.520128     0.340718     248.39
 C       5.477589    -0.969491     1.330065     121.95
 H       5.167142    -0.215943     2.032207      26.55
 H       6.344914    -0.577779     0.869438      28.86
 H       5.899541    -1.987801     1.742949      25.33
 C       3.546034    -0.663532    -1.574687      15.42
 O       3.817055    -1.861516    -2.273353     207.52
 H       3.826539    -2.558092    -1.677131      27.12
 C       3.178264     0.415382    -2.496146      31.23
 H       3.478094     0.422087    -3.557803      21.08
 C       2.806818     1.820187    -0.487600      71.70
 C       2.115177     3.125439     0.047496      91.79
 H       2.453954     4.109686    -0.635301      20.19
 O       2.415735     3.412488     1.535120     309.06
 H       3.240012     3.830695     1.611620      30.07
 C       0.548438     3.098724    -0.080721      54.97
 H       0.298689     2.971390    -1.140537      21.85
 C      -0.166904     4.399004     0.445780      85.67
 O       0.223987     5.674877    -0.406540     221.41
 H       0.144515     5.558361    -1.313640      31.79
 H      -0.012336     4.861378     1.550170      22.91
 H      -1.264901     4.355053     0.318408      23.37
 C      -1.100310    -1.538816    -0.359554      59.25
 H      -0.700357    -2.551547    -0.593527      17.76
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 C      -2.987366     0.093173    -0.691788      65.12
 H      -4.022629     0.143379    -0.938189      21.86
 C      -2.163962     1.181433    -0.240620      -3.50
 O      -2.394792     2.508661     0.043732     187.61
 C      -3.933983     2.758078     0.225224     113.04
 H      -4.343987     3.043130    -0.698666      25.91
 H      -4.058530     2.136396     0.975611      27.36
 H      -3.863476     3.784816     0.801472      25.37
 C      -0.720662     0.833525     0.160828      -6.49
 O       0.063970     1.803868     0.624750     165.07
 C      -0.136280    -0.535246    -0.094899      27.68
 H       0.963752    -0.324634     0.337901      17.01
 C      -2.395797    -1.149493    -0.729379      16.69
 C      -3.256363    -2.373345    -1.330075      71.94
 H      -4.208265    -2.095821    -1.665557      25.55
 O      -2.547757    -2.910872    -2.324377     220.16
 H      -2.965400    -3.934123    -2.387689      15.32
 C      -3.552350    -3.358804    -0.026655      90.21
 H      -2.645724    -3.573207     0.579485      23.37
 O      -4.392804    -2.610307     0.843087     357.86
 H      -3.880033    -2.252195     1.641228      27.14
 C      -4.276487    -4.574218    -0.591821     111.95
 O      -3.385913    -5.229354    -1.502195     341.71
 H      -2.894220    -5.971669    -1.110615      27.55
 H      -4.999906    -4.334648    -1.255920      29.22
 H      -4.612144    -5.143820     0.208964      28.38
55
name = lig-etoh-frame_59
 C       2.661619     1.704546    -2.023075      60.24
 H       2.871678     2.521714    -2.698574      26.10
 C       3.559330     0.850436     0.300930      64.66
 H       3.431966     1.210833     1.381851      18.57
 C       3.709853    -0.465630    -0.223231      13.76
 O       4.612223    -1.509952     0.344172     205.43
 C       5.485803    -1.019173     1.387991     113.55
 H       5.052537    -0.188954     2.004037      25.49
 H       6.465721    -0.709149     0.746977      25.28
 H       5.894765    -1.807786     1.981432      27.31
 C       3.530061    -0.739642    -1.659357      -1.99
 O       3.827726    -1.860106    -2.283058     148.86
 H       3.785689    -2.783419    -1.640564      20.87
 C       3.171218     0.467613    -2.467436      28.71
 H       3.387957     0.209337    -3.572105      19.75
 C       2.840237     1.871960    -0.441141      38.10
 C       2.137512     3.120906     0.039375      95.90
 H       2.447992     3.943594    -0.485560      22.33
 O       2.382991     3.424709     1.540171     284.77
 H       3.397748     3.763435     1.545835      26.12
 C       0.505898     3.151995    -0.132932      44.40
 H       0.263566     2.767863    -1.143094      20.79
 C      -0.200225     4.391481     0.468775      93.20
 O       0.248532     5.675655    -0.390726     190.99
 H       0.127926     5.601843    -1.415573      27.16
 H       0.292297     4.492557     1.403861      24.87
 H      -1.260336     4.160309     0.298511      22.48
 C      -1.027643    -1.554197    -0.435626      32.39
 H      -0.811458    -2.587523    -0.618886      16.33
 C      -2.974910     0.134226    -0.690198      51.04
 H      -4.107620     0.075801    -0.984347      21.32
 C      -2.149623     1.076773    -0.188974       4.32
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 O      -2.435063     2.515474     0.040241     150.99
 C      -3.887074     2.852885     0.186982      78.80
 H      -4.698867     2.864214    -0.754064      24.06
 H      -4.394079     1.799650     1.139568      21.32
 H      -3.930033     3.835792     0.627962      24.84
 C      -0.678191     0.810871     0.054633      27.60
 O       0.070440     1.832604     0.684941     134.69
 C      -0.163245    -0.499870    -0.067323      44.07
 H       0.865068    -0.879343     0.182623      19.67
 C      -2.380332    -1.138554    -0.771820      25.65
 C      -3.309431    -2.330123    -1.202930      49.67
 H      -4.433334    -1.980826    -1.424679      23.13
 O      -2.583590    -2.899824    -2.365455     237.12
 H      -2.741960    -3.805886    -2.561262      20.41
 C      -3.491720    -3.390133    -0.041904     102.41
 H      -2.643513    -3.471990     0.634756      24.45
 O      -4.377608    -2.573887     0.815339     338.32
 H      -3.830634    -2.213579     1.498152      29.36
 C      -4.338860    -4.530825    -0.608285      67.39
 O      -3.382531    -5.314573    -1.531897     306.57
 H      -2.780411    -6.089709    -1.162980      25.60
 H      -5.310409    -4.008300    -1.177131      25.88
 H      -4.779663    -5.306197     0.189624      25.07
55
name = lig-etoh-frame_60
 C       2.692997     1.708822    -1.911539      46.63
 H       2.559656     2.601359    -2.560666      24.35
 C       3.518914     0.980729     0.356025      83.75
 H       3.300709     0.966794     1.405780      20.13
 C       3.735312    -0.424645    -0.288192      -5.54
 O       4.611894    -1.482534     0.355855     183.46
 C       5.535379    -1.058997     1.413950     114.41
 H       4.994856    -0.239333     1.928036      26.52
 H       6.398261    -0.649498     0.909608      28.03
 H       5.753647    -1.801072     2.283792      25.94
 C       3.483238    -0.700788    -1.689458      15.03
 O       3.843543    -1.908437    -2.308136     212.90
 H       3.852668    -2.621702    -1.653186      25.93
 C       3.163539     0.458519    -2.450421      25.59
 H       3.187592     0.199224    -3.470574      19.72
 C       2.863405     1.896666    -0.493521      28.61
 C       2.129302     3.117230     0.095496     102.57
 H       2.579774     4.075348    -0.532874      19.08
 O       2.364893     3.438071     1.509092     307.42
 H       3.367010     3.558206     1.520303      28.69
 C       0.502045     3.128625    -0.167462      54.48
 H       0.225789     2.857362    -1.223750      20.34
 C      -0.190782     4.391729     0.408243      98.59
 O       0.261414     5.654444    -0.346229     196.17
 H       0.150695     5.389601    -1.386965      26.60
 H       0.382725     4.345476     1.407727      23.75
 H      -1.267123     4.177038     0.493692      23.68
 C      -1.013758    -1.512888    -0.536934      34.99
 H      -0.772112    -2.632391    -0.560315      17.70
 C      -2.977546     0.128542    -0.693965      42.11
 H      -3.963845     0.314699    -0.913314      23.14
 C      -2.059250     1.063374    -0.122117      -5.95
 O      -2.513882     2.491575     0.020385     205.75
 C      -3.866476     2.865890     0.188343     142.52
 H      -4.486911     2.565686    -0.602475      27.72
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 H      -4.453053     2.355483     0.658759      31.26
 H      -3.966382     3.899366     0.555728      26.71
 C      -0.673645     0.818916    -0.036636      25.14
 O       0.079874     1.873994     0.738795     123.99
 C      -0.188269    -0.491032    -0.035958      45.83
 H       0.773279    -1.020092     0.038549      19.02
 C      -2.377166    -1.207398    -0.820714      11.48
 C      -3.328833    -2.293126    -1.080050      83.44
 H      -4.288520    -1.935098    -1.258940      23.74
 O      -2.622833    -2.869142    -2.420182     181.64
 H      -2.729794    -3.868025    -2.519059      17.04
 C      -3.472316    -3.357406    -0.054868     104.92
 H      -2.495785    -3.761540     0.432199      19.70
 O      -4.386040    -2.542432     0.800226     324.58
 H      -3.679645    -2.185278     1.501070      22.95
 C      -4.382060    -4.536463    -0.611279      94.77
 O      -3.402376    -5.395644    -1.578993     306.09
 H      -2.983980    -5.919549    -0.860659      27.42
 H      -5.144350    -4.029364    -1.035684      31.50
 H      -4.791616    -5.214136     0.022943      30.07
55
name = lig-etoh-frame_61
 C       2.787446     1.686251    -1.806224      40.16
 H       2.132051     2.453433    -2.328365      20.08
 C       3.445216     1.014239     0.352714      85.80
 H       3.334923     0.812543     1.473645      20.27
 C       3.819302    -0.357745    -0.322520       0.68
 O       4.582288    -1.447273     0.358422     187.23
 C       5.548420    -1.068841     1.448862     110.18
 H       5.088149    -0.212340     1.941336      27.57
 H       6.569566    -0.603213     1.100555      26.67
 H       5.553129    -1.885102     2.195299      26.61
 C       3.462617    -0.630620    -1.659457      22.47
 O       3.852121    -1.938275    -2.338803     195.57
 H       3.968922    -2.525674    -1.570636      25.85
 C       3.126881     0.443481    -2.440609      43.78
 H       2.915307     0.374119    -3.602287      19.44
 C       2.858553     1.929430    -0.522657      35.61
 C       2.108942     3.167380     0.117711     126.83
 H       2.503362     3.966514    -0.437650      24.23
 O       2.353554     3.434969     1.462816     318.18
 H       3.326515     3.509094     1.578847      31.53
 C       0.531693     3.056999    -0.173141      76.68
 H       0.288286     3.006394    -1.231162      20.56
 C      -0.128131     4.383017     0.347080     112.00
 O       0.254431     5.594525    -0.301232     279.46
 H       0.272176     5.345274    -1.155555      35.27
 H       0.189785     4.545374     1.416513      24.89
 H      -1.214485     4.396753     0.630828      24.52
 C      -1.053224    -1.466239    -0.630275      53.81
 H      -0.621163    -2.416653    -0.538995      20.33
 C      -2.899876     0.083166    -0.672744      37.41
 H      -3.969592     0.573684    -0.833720      20.75
 C      -2.030842     1.117493    -0.102289      -5.28
 O      -2.555750     2.434306     0.008676     177.07
 C      -3.844810     2.868875     0.152771      88.49
 H      -4.271184     2.644611    -1.025066      21.93
 H      -4.753896     2.320496     1.176716      20.70
 H      -3.909971     4.040860     0.327086      23.01
 C      -0.642317     0.885392    -0.034424      11.45
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 O       0.078914     1.913774     0.744739     174.18
 C      -0.213788    -0.524627    -0.046518      26.56
 H       1.005103    -0.660390     0.066985      17.08
 C      -2.397151    -1.232515    -0.844304      30.36
 C      -3.284792    -2.300904    -1.061539      83.61
 H      -4.326854    -1.868600    -1.337750      21.57
 O      -2.688298    -2.833592    -2.467147     161.65
 H      -2.849777    -3.872749    -2.229084      13.84
 C      -3.496052    -3.353853    -0.052450     109.17
 H      -2.616963    -3.882479     0.216715      20.46
 O      -4.369966    -2.522910     0.824365     339.38
 H      -3.799684    -2.222844     1.572338      26.39
 C      -4.340737    -4.546025    -0.636416      66.40
 O      -3.461011    -5.457016    -1.590905     287.09
 H      -3.112514    -5.788501    -0.712266      24.00
 H      -5.216219    -4.063133    -1.340446      25.65
 H      -4.808970    -5.273307     0.209659      26.59
55
name = lig-etoh-frame_62
 C       2.849341     1.660606    -1.816625      32.24
 H       2.052090     2.187593    -2.263535      20.70
 C       3.393867     0.906375     0.324042      44.25
 H       3.435240     1.023018     1.378288      20.56
 C       3.924502    -0.255422    -0.297271      20.69
 O       4.548658    -1.388542     0.357077     212.50
 C       5.520477    -1.042444     1.465488     108.24
 H       5.183015    -0.152024     2.096678      25.24
 H       6.638159    -0.904644     1.258494      26.48
 H       5.509016    -2.015578     1.994736      26.15
 C       3.509370    -0.620787    -1.647008      12.13
 O       3.835965    -1.919271    -2.343227     141.30
 H       4.231291    -2.490751    -1.437428      21.91
 C       3.049688     0.468992    -2.468396      56.49
 H       2.763965     0.463759    -3.439056      24.77
 C       2.843398     1.979605    -0.409743      43.47
 C       2.082141     3.198109     0.081725     103.09
 H       2.427795     4.172945    -0.573044      22.29
 O       2.338193     3.421662     1.439702     282.94
 H       3.390691     3.617533     1.600511      25.33
 C       0.578289     3.008505    -0.117913      74.97
 H       0.392777     2.926279    -1.251538      19.70
 C      -0.082832     4.373966     0.370115     109.44
 O       0.252717     5.539259    -0.265872     213.83
 H       0.461340     5.437223    -1.342970      26.88
 H       0.201106     4.641637     1.413565      24.33
 H      -1.181328     4.405716     0.370734      24.19
 C      -1.049137    -1.429466    -0.678292      54.59
 H      -0.533867    -2.455510    -0.700264      19.99
 C      -2.809093     0.093466    -0.622055      65.64
 H      -3.809404     0.347764    -0.762353      24.48
 C      -2.057271     1.159232    -0.146188       9.65
 O      -2.536813     2.374529     0.028161     226.23
 C      -3.924834     2.840153     0.092850     134.54
 H      -4.229240     2.926159    -0.878439      26.85
 H      -4.280139     2.569049     0.932319      28.87
 H      -3.731948     3.905364     0.120703      26.46
 C      -0.611153     0.946502     0.054163      11.07
 O       0.077232     1.948260     0.696645     238.72
 C      -0.195512    -0.464988    -0.092696      31.09
 H       0.805845    -0.419303     0.133371      18.01
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 C      -2.417807    -1.178349    -0.832537      33.52
 C      -3.269189    -2.327871    -1.184901      88.50
 H      -4.248909    -1.943814    -1.425220      22.82
 O      -2.785329    -2.828314    -2.471801     294.31
 H      -2.823863    -3.720889    -2.314606      20.86
 C      -3.568085    -3.370101    -0.061662      76.25
 H      -2.573949    -3.812071     0.412819      19.04
 O      -4.344064    -2.532009     0.870325     356.00
 H      -3.848696    -2.323330     1.731579      24.44
 C      -4.340401    -4.554900    -0.694592     110.94
 O      -3.544436    -5.490174    -1.543265     303.87
 H      -2.830872    -6.024217    -0.919721      25.20
 H      -5.064279    -4.365630    -1.402526      28.61
 H      -4.679927    -5.034499     0.142925      28.76
55
name = lig-etoh-frame_63
 C       2.841112     1.686150    -1.816063      31.33
 H       2.166123     2.321953    -2.510765      20.41
 C       3.358496     0.814470     0.327139      68.46
 H       3.600937     1.177392     1.380680      21.99
 C       4.010585    -0.208465    -0.304842      31.42
 O       4.532951    -1.294836     0.371478     230.59
 C       5.475329    -1.042277     1.485631     115.18
 H       5.217032    -0.289773     2.174436      25.97
 H       6.558843    -1.072472     1.110390      26.10
 H       5.449362    -2.090929     1.961187      25.42
 C       3.601726    -0.617447    -1.683514       2.13
 O       3.821575    -1.864088    -2.280322     237.78
 H       4.345544    -2.347500    -1.742961      28.18
 C       2.997900     0.455470    -2.450755      46.11
 H       2.614471     0.327019    -3.561794      22.76
 C       2.853876     1.974077    -0.342698      65.76
 C       2.096821     3.224253     0.020124     105.23
 H       2.226553     4.099612    -0.582678      23.76
 O       2.342175     3.422871     1.450919     329.58
 H       3.228175     3.718707     1.457075      29.72
 C       0.613986     3.024139    -0.066672      80.10
 H       0.432494     2.756600    -1.077450      22.40
 C      -0.085503     4.337953     0.427320     102.77
 O       0.286744     5.533643    -0.292679     251.75
 H       0.555760     5.497668    -1.266489      28.79
 H       0.254833     4.487648     1.527917      23.17
 H      -1.131937     4.076438     0.112977      22.44
 C      -0.979860    -1.413185    -0.682454      41.17
 H      -0.678505    -2.395638    -0.973865      20.41
 C      -2.784412     0.138313    -0.568523      59.93
 H      -3.939727     0.132171    -0.732902      20.11
 C      -2.023164     1.163453    -0.204479      32.53
 O      -2.505750     2.363417     0.062329     162.21
 C      -3.932743     2.857759    -0.021770      74.29
 H      -4.710831     2.789679    -0.989742      22.65
 H      -4.386401     2.455083     1.267720      19.52
 H      -3.515677     3.954675     0.164905      22.53
 C      -0.661727     0.952942     0.146434      25.45
 O       0.090182     1.972293     0.651157     259.60
 C      -0.193366    -0.308029    -0.158825      48.98
 H       0.989876    -0.588862     0.264394      16.41
 C      -2.377371    -1.157126    -0.816172      19.60
 C      -3.286962    -2.337416    -1.328395      69.04
 H      -4.377276    -1.944625    -1.490863      21.77
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 O      -2.875531    -2.837998    -2.480508     287.44
 H      -2.768678    -3.901535    -2.572699      17.32
 C      -3.601918    -3.357451    -0.084735      88.61
 H      -2.794376    -3.602100     0.526136      23.22
 O      -4.331897    -2.563835     0.913137     328.35
 H      -3.724577    -2.555264     1.770311      23.01
 C      -4.325550    -4.586368    -0.736515      83.60
 O      -3.595361    -5.530515    -1.472926     353.75
 H      -2.869982    -6.004833    -1.228072      32.59
 H      -5.235479    -4.370459    -1.488256      24.36
 H      -4.820120    -5.083016     0.248579      24.24
55
name = lig-etoh-frame_64
 C       2.763699     1.749409    -1.809270      55.63
 H       2.615360     2.573741    -2.496630      22.34
 C       3.340961     0.839014     0.383044      58.00
 H       3.723801     0.970823     1.389490      23.97
 C       4.052990    -0.232690    -0.377912      23.96
 O       4.539124    -1.207755     0.408187     229.77
 C       5.435026    -1.111502     1.490354     112.68
 H       5.212915    -0.284225     2.269904      24.77
 H       6.424289    -0.951618     0.882930      24.92
 H       5.366236    -2.001924     2.071235      26.53
 C       3.700275    -0.559272    -1.719538      18.51
 O       3.801701    -1.790496    -2.219559     215.90
 H       4.584098    -2.358761    -1.801435      23.66
 C       2.975374     0.405078    -2.421643      31.79
 H       2.659293     0.135769    -3.391362      22.27
 C       2.876145     1.912790    -0.422586      43.69
 C       2.128781     3.195632     0.026343      89.49
 H       2.329222     4.147204    -0.681971      21.14
 O       2.348077     3.444963     1.463772     273.98
 H       3.325759     3.861187     1.474496      24.69
 C       0.633776     3.071393    -0.060803      64.12
 H       0.352195     2.808125    -1.158953      20.04
 C      -0.101316     4.280489     0.444406     104.96
 O       0.333184     5.556766    -0.315514     243.34
 H       0.527682     5.305393    -1.223682      30.62
 H       0.059769     4.342215     1.483743      25.89
 H      -1.105641     3.920588     0.236408      23.26
 C      -0.923603    -1.360813    -0.672498      44.72
 H      -0.563646    -2.328316    -1.126959      16.94
 C      -2.869245     0.117738    -0.552276      46.93
 H      -3.963096     0.247047    -0.623347      16.91
 C      -1.978047     1.175113    -0.235573      29.79
 O      -2.501083     2.409416     0.084415     210.69
 C      -3.918184     2.889719    -0.063671     132.28
 H      -4.650709     2.478414    -0.654815      26.87
 H      -4.475046     2.548143     0.736733      27.67
 H      -3.778344     3.894601     0.085096      27.45
 C      -0.722936     0.952872     0.200261      20.43
 O       0.108987     1.966794     0.670015     251.86
 C      -0.121750    -0.230600    -0.207034      61.89
 H       0.724221    -0.562864     0.079991      20.62
 C      -2.292606    -1.182304    -0.825474       8.67
 C      -3.358721    -2.295677    -1.349242      74.11
 H      -4.346322    -1.855276    -1.492417      23.06
 O      -2.921703    -2.891102    -2.566338     290.79
 H      -2.890601    -3.921354    -2.615264      19.05
 C      -3.622728    -3.306992    -0.144306      70.37
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 H      -2.647515    -3.679848     0.427424      20.51
 O      -4.339007    -2.615444     0.942420     357.92
 H      -3.725780    -2.583493     1.651336      27.09
 C      -4.368251    -4.634173    -0.699096     107.15
 O      -3.641898    -5.571527    -1.455169     319.89
 H      -2.760420    -5.958312    -0.968763      25.98
 H      -5.160047    -4.199714    -1.291876      27.73
 H      -4.912896    -5.120788     0.045466      27.78
55
name = lig-etoh-frame_65
 C       2.697544     1.749890    -1.857599      69.38
 H       2.922801     2.742001    -2.367490      20.38
 C       3.390150     0.873644     0.377968      33.62
 H       3.619594     0.813923     1.455381      21.53
 C       4.030178    -0.204415    -0.388702       8.89
 O       4.538857    -1.186482     0.439109     236.71
 C       5.417799    -1.138585     1.488572     119.56
 H       5.268368    -0.297065     2.125584      27.01
 H       6.417008    -0.876901     1.078876      26.55
 H       5.371778    -2.118131     2.150599      24.65
 C       3.777872    -0.462081    -1.716125      39.73
 O       3.795530    -1.764450    -2.178207     195.48
 H       4.751874    -2.205656    -1.872667      23.46
 C       2.967866     0.415374    -2.374417      38.43
 H       2.685258     0.050027    -3.411656      22.91
 C       2.873820     1.872861    -0.511833      37.23
 C       2.181812     3.156417     0.069528     108.42
 H       2.613467     3.956800    -0.547930      21.96
 O       2.382294     3.489951     1.464718     301.25
 H       3.307956     3.817522     1.643197      27.31
 C       0.631382     3.090845    -0.121507      62.51
 H       0.360264     3.082644    -1.143483      20.29
 C      -0.121190     4.250393     0.415804      93.29
 O       0.365792     5.561037    -0.312052     182.53
 H       0.419145     5.040106    -1.289350      26.05
 H      -0.083967     4.417037     1.605409      22.63
 H      -1.234496     4.134911     0.372789      22.17
 C      -0.870725    -1.296872    -0.682802      47.81
 H      -0.247610    -2.122343    -1.032889      17.30
 C      -2.925208     0.064100    -0.552988      44.60
 H      -3.981464     0.392276    -0.569485      15.77
 C      -2.060678     1.192960    -0.239312       5.15
 O      -2.516481     2.489049     0.093882     207.41
 C      -3.858166     2.894184    -0.070242      90.46
 H      -4.358632     2.234927    -1.018380      22.08
 H      -4.731346     2.511445     0.891550      21.15
 H      -4.173678     4.100978    -0.224562      22.52
 C      -0.691787     0.968924     0.210888       5.36
 O       0.128222     1.941003     0.741240     207.09
 C      -0.095748    -0.240518    -0.255445      29.36
 H       1.182530    -0.468530     0.003536      14.49
 C      -2.282126    -1.192511    -0.858706      21.99
 C      -3.397699    -2.247655    -1.298227      63.02
 H      -4.340957    -1.654023    -1.545909      21.79
 O      -2.953200    -2.950674    -2.675898     256.12
 H      -3.111283    -3.866833    -2.464206      21.28
 C      -3.608443    -3.292575    -0.185417      83.50
 H      -2.630454    -3.681957    -0.040525      21.45
 O      -4.364978    -2.684076     0.932491     335.19
 H      -3.681171    -2.398921     1.733629      21.77
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 C      -4.433346    -4.631426    -0.629585      83.31
 O      -3.645260    -5.624216    -1.456319     330.64
 H      -3.088650    -5.755828    -0.629108      25.92
 H      -5.190327    -4.113106    -1.343890      25.74
 H      -5.013617    -5.238254     0.193992      25.43
55
name = lig-etoh-frame_66
 C       2.680999     1.718356    -1.938773      61.46
 H       2.759967     2.661214    -2.440159      19.67
 C       3.478876     0.898618     0.298327      40.75
 H       3.275567     0.899864     1.412706      19.61
 C       3.997678    -0.137156    -0.278407      19.45
 O       4.520100    -1.227354     0.428881     228.36
 C       5.437490    -1.136279     1.513434     116.39
 H       5.180049    -0.219265     2.172763      25.08
 H       6.623937    -1.002150     1.373100      25.46
 H       5.409456    -2.054636     1.973248      27.56
 C       3.808289    -0.395303    -1.694497      44.04
 O       3.824310    -1.761742    -2.150589     254.63
 H       4.617759    -2.046855    -1.959614      29.83
 C       2.963182     0.481537    -2.391538      52.69
 H       2.723288     0.151567    -3.430094      24.80
 C       2.845252     1.866161    -0.492286      56.43
 C       2.247428     3.115550     0.118795     107.45
 H       2.781794     3.959966    -0.494913      19.95
 O       2.419068     3.528341     1.475217     305.77
 H       3.367883     3.721790     1.607652      29.49
 C       0.628843     3.096451    -0.151923      45.10
 H       0.397276     3.056840    -1.290417      19.30
 C      -0.159756     4.305326     0.432446     109.85
 O       0.378285     5.504644    -0.311322     242.89
 H       0.386814     5.352326    -1.237212      32.53
 H       0.067225     4.494057     1.405300      27.34
 H      -1.229433     4.387712     0.225213      24.59
 C      -0.830461    -1.265409    -0.726200      39.87
 H      -0.147031    -2.102913    -0.925608      17.41
 C      -2.915225     0.052162    -0.554214      42.00
 H      -4.073162     0.268573    -0.632450      16.75
 C      -2.156801     1.199439    -0.187310       0.72
 O      -2.530654     2.580006     0.105965     223.56
 C      -3.903798     2.861847    -0.104460     139.20
 H      -3.858490     2.464976    -1.069346      25.26
 H      -4.431523     2.612682     0.784481      26.56
 H      -4.095639     3.780957    -0.455113      28.11
 C      -0.649678     0.981295     0.157354      -6.79
 O       0.149838     1.922312     0.808674     161.33
 C      -0.022599    -0.242893    -0.248740      29.54
 H       0.917430    -0.187697    -0.245867      18.21
 C      -2.332781    -1.184839    -0.896841      30.21
 C      -3.392121    -2.203071    -1.282812      65.54
 H      -4.255930    -1.570949    -1.594459      22.62
 O      -2.992982    -2.989428    -2.745424     163.07
 H      -3.343752    -3.941283    -2.339673      17.01
 C      -3.615052    -3.319525    -0.214713      67.13
 H      -2.488031    -3.652834    -0.180247      17.92
 O      -4.362949    -2.759165     0.918881     339.24
 H      -3.854568    -2.268010     1.575034      26.50
 C      -4.534187    -4.589761    -0.595831      87.27
 O      -3.650315    -5.643311    -1.414406     286.31
 H      -3.140132    -6.004668    -0.661232      25.54
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 H      -5.306262    -4.322414    -1.356097      26.80
 H      -4.892703    -5.080767     0.296794      27.22
55
name = lig-etoh-frame_67
 C       2.690275     1.743116    -1.934625      28.19
 H       2.250903     2.508859    -2.705252      17.37
 C       3.504841     1.008290     0.284237      53.32
 H       3.125654     1.088431     1.262313      18.57
 C       4.024696    -0.180786    -0.221046      16.11
 O       4.512868    -1.289236     0.402646     226.85
 C       5.482534    -1.089509     1.562319     107.23
 H       5.074935    -0.388505     2.255682      26.48
 H       6.521921    -1.070148     1.324595      27.11
 H       5.325135    -2.172571     2.042661      24.76
 C       3.777892    -0.373476    -1.645353      30.22
 O       3.846276    -1.731901    -2.130959     170.49
 H       4.845120    -2.142882    -1.934281      22.82
 C       3.002403     0.503337    -2.477506      45.96
 H       2.770662     0.303850    -3.497695      26.25
 C       2.808193     1.882791    -0.475588     112.63
 C       2.275790     3.124141     0.129831     129.66
 H       2.667607     3.974783    -0.496583      24.80
 O       2.457661     3.548263     1.501503     284.43
 H       3.533127     3.655669     1.486444      29.78
 C       0.628170     3.107839    -0.133326      46.89
 H       0.468412     2.758568    -1.131648      18.78
 C      -0.169590     4.398373     0.390656     103.93
 O       0.394262     5.463881    -0.297949     234.05
 H       0.359565     5.562445    -1.311314      28.79
 H       0.286808     4.564062     1.505400      23.81
 H      -1.233534     4.346845     0.145585      23.63
 C      -0.833540    -1.276630    -0.789864      37.59
 H      -0.387621    -2.295225    -0.961616      20.58
 C      -2.912794     0.099289    -0.558135      43.02
 H      -3.936586     0.028606    -0.732139      19.26
 C      -2.152109     1.219981    -0.079413     -13.32
 O      -2.508720     2.637295     0.130353     177.37
 C      -3.927347     2.820554    -0.202202      83.05
 H      -4.092918     2.285811    -1.230442      23.42
 H      -4.564732     2.481171     0.920172      20.55
 H      -3.910452     4.036695    -0.471841      22.56
 C      -0.665363     0.996644     0.080541      17.71
 O       0.164644     1.916707     0.832837     146.16
 C      -0.037945    -0.190155    -0.227672      24.08
 H       1.247911    -0.100073    -0.424435      12.28
 C      -2.326289    -1.167103    -0.919181      17.02
 C      -3.362194    -2.186880    -1.333668      58.36
 H      -4.289907    -1.668639    -1.589223      21.92
 O      -3.054373    -3.016987    -2.745458     230.76
 H      -3.292390    -3.929556    -2.614318      21.74
 C      -3.629095    -3.352459    -0.248217      80.82
 H      -2.678768    -3.696862     0.097648      19.59
 O      -4.359587    -2.839051     0.888643     319.21
 H      -3.795320    -2.246360     1.494414      23.46
 C      -4.574106    -4.558785    -0.610156      75.93
 O      -3.680704    -5.631660    -1.338389     266.66
 H      -3.046202    -6.333668    -0.869904      25.40
 H      -5.494378    -4.478710    -1.257572      25.42
 H      -4.861989    -4.914807     0.433113      25.35
55
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name = lig-etoh-frame_68
 C       2.685312     1.795804    -1.918793      38.37
 H       1.871781     2.178188    -2.472891      20.45
 C       3.513081     1.097219     0.325822      58.52
 H       3.277287     1.258615     1.452601      14.15
 C       4.047359    -0.235410    -0.249555       9.54
 O       4.537592    -1.349623     0.402843     233.88
 C       5.466426    -1.113150     1.617304      99.06
 H       5.071039    -0.371012     2.359998      26.03
 H       6.537828    -0.905888     1.049744      24.20
 H       5.365131    -2.001319     2.122121      27.16
 C       3.714575    -0.408423    -1.600472      15.99
 O       3.891553    -1.691259    -2.115959     202.14
 H       4.796370    -2.164142    -1.876597      23.85
 C       3.086984     0.518183    -2.533627      72.39
 H       2.865761     0.333929    -3.674547      24.10
 C       2.780894     1.944881    -0.530969      86.93
 C       2.207791     3.194922     0.115137     140.33
 H       2.522250     4.051712    -0.564954      26.50
 O       2.525527     3.545143     1.518588     312.81
 H       3.457205     3.742871     1.564367      36.26
 C       0.639183     3.097032    -0.038607      57.82
 H       0.442838     2.603469    -1.030024      17.97
 C      -0.124932     4.442482     0.337317     121.69
 O       0.437754     5.495308    -0.299918     247.36
 H       0.211232     5.488476    -1.372163      26.43
 H       0.064114     4.538621     1.333863      28.36
 H      -1.215732     4.196481     0.329184      23.82
 C      -0.879724    -1.301689    -0.841622      38.90
 H      -0.614345    -2.315092    -1.063816      20.31
 C      -2.881530     0.162664    -0.560737      44.07
 H      -4.067553     0.056415    -0.808953      19.55
 C      -2.080945     1.250472     0.030676       1.40
 O      -2.494213     2.628794     0.145358     188.72
 C      -3.935729     2.820097    -0.304945     127.35
 H      -4.522357     2.190751    -0.987259      25.77
 H      -4.640594     2.506899     0.473115      26.86
 H      -3.958568     3.817717    -0.247582      27.63
 C      -0.708357     1.045191     0.054111      17.16
 O       0.161236     1.925469     0.809205     204.96
 C      -0.050945    -0.172642    -0.265609      27.91
 H       0.932253    -0.254930    -0.316213      16.55
 C      -2.251845    -1.121942    -0.927458      10.69
 C      -3.325774    -2.251443    -1.420905      52.94
 H      -4.396473    -1.806851    -1.541433      21.12
 O      -3.107250    -3.001560    -2.715370     269.38
 H      -3.231473    -3.993738    -2.703104      21.71
 C      -3.665111    -3.361167    -0.281096      85.28
 H      -2.804007    -3.889602     0.291293      16.99
 O      -4.367046    -2.894145     0.861843     289.30
 H      -3.658448    -2.401050     1.443463      22.06
 C      -4.537657    -4.586456    -0.621981      83.89
 O      -3.738247    -5.609266    -1.280184     306.68
 H      -3.144773    -6.191451    -0.762457      28.59
 H      -5.568598    -4.514320    -1.141923      25.88
 H      -4.848771    -4.817598     0.432876      25.61
55
name = lig-etoh-frame_69
 C       2.668213     1.763287    -1.936061      29.60
 H       1.709497     2.299687    -2.219317      18.41
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 C       3.529605     1.103520     0.364697      36.23
 H       3.707895     1.351483     1.381761      19.71
 C       4.015593    -0.190989    -0.257272       8.69
 O       4.578555    -1.395463     0.433501     220.32
 C       5.434874    -1.125415     1.616360     114.25
 H       5.174013    -0.239839     2.230342      26.59
 H       6.283064    -0.774201     1.204122      28.82
 H       5.568357    -2.127534     2.253008      25.04
 C       3.652444    -0.463496    -1.609508      23.97
 O       3.939357    -1.672555    -2.120944     241.33
 H       4.660676    -2.034476    -1.744588      28.89
 C       3.183109     0.569724    -2.526101      42.47
 H       3.057745     0.278216    -3.496517      19.68
 C       2.800584     2.023310    -0.552508      37.17
 C       2.105322     3.290937     0.099853     108.23
 H       2.351559     4.202177    -0.576976      22.65
 O       2.566456     3.524730     1.514528     282.09
 H       3.580384     3.904537     1.585224      27.54
 C       0.646237     3.062733     0.065643      89.43
 H       0.420513     2.888834    -1.009619      17.14
 C      -0.086238     4.390962     0.310635     104.93
 O       0.479311     5.578246    -0.350752     271.08
 H       0.255471     5.393404    -1.189190      34.32
 H      -0.051362     4.607226     1.514411      23.69
 H      -1.164963     4.265713     0.276096      24.16
 C      -0.908371    -1.291132    -0.859711      41.70
 H      -0.495171    -2.302409    -1.168763      19.42
 C      -2.842087     0.205158    -0.563315      73.22
 H      -3.816986     0.408808    -0.688041      23.88
 C      -2.063846     1.270829     0.075690       5.98
 O      -2.521709     2.568009     0.143001     196.34
 C      -3.925172     2.809624    -0.359238      94.29
 H      -4.458059     2.245505    -1.215768      25.16
 H      -4.794620     2.504590     0.580300      22.91
 H      -4.157769     3.999596    -0.318658      23.64
 C      -0.677991     1.072588     0.089564      37.00
 O       0.143019     1.947966     0.772965     254.98
 C      -0.156622    -0.214488    -0.344817      22.69
 H       1.093656    -0.399260    -0.129975      14.36
 C      -2.246365    -1.056460    -0.947747       3.54
 C      -3.314841    -2.357694    -1.474938      75.68
 H      -4.243819    -1.829578    -1.524617      23.18
 O      -3.139156    -2.955494    -2.686080     275.04
 H      -3.142392    -4.027480    -2.494448      19.12
 C      -3.677422    -3.386957    -0.292258      95.26
 H      -2.780564    -3.923482    -0.001398      19.39
 O      -4.378708    -2.898816     0.851050     344.45
 H      -3.755300    -2.582379     1.483116      26.74
 C      -4.498375    -4.637377    -0.617172      94.55
 O      -3.806261    -5.594908    -1.251012     328.53
 H      -3.250327    -5.872190    -0.454801      27.63
 H      -5.407483    -4.414431    -1.183080      26.47
 H      -4.817687    -4.981608     0.385409      26.63
55
name = lig-etoh-frame_70
 C       2.619563     1.719439    -1.925021      51.80
 H       1.992759     2.508951    -2.351682      21.52
 C       3.557761     1.075376     0.332794      73.03
 H       4.098115     1.433988     1.279318      22.83
 C       3.949481    -0.114851    -0.222535       0.17
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 O       4.605602    -1.404588     0.466169     208.85
 C       5.390744    -1.136757     1.606544     117.53
 H       5.013511    -0.272741     2.164162      25.44
 H       6.529435    -0.664828     1.297010      24.69
 H       5.723298    -1.980789     2.161425      26.44
 C       3.614890    -0.465121    -1.624852      15.94
 O       3.976724    -1.680483    -2.162617     142.39
 H       4.718123    -2.038873    -1.347034      18.83
 C       3.266207     0.609222    -2.453959      43.94
 H       3.177478     0.213874    -3.570553      18.90
 C       2.869420     2.076625    -0.510562      19.09
 C       2.082671     3.357088     0.104235      99.68
 H       2.181468     4.280265    -0.462717      18.72
 O       2.590907     3.509702     1.493884     316.45
 H       3.484230     3.882116     1.372855      30.37
 C       0.622849     3.070664     0.100988      96.41
 H       0.444376     3.121809    -1.005640      16.13
 C      -0.072021     4.360319     0.387084      99.42
 O       0.503565     5.638559    -0.388543     134.77
 H       0.397417     5.417143    -1.459935      25.66
 H      -0.001522     4.695868     1.357911      25.20
 H      -1.108782     4.405165    -0.078214      21.75
 C      -0.910930    -1.274262    -0.872122      46.38
 H      -0.315448    -2.106619    -1.164963      18.34
 C      -2.766910     0.234463    -0.547215      52.43
 H      -3.885015     0.679973    -0.625820      17.71
 C      -2.070710     1.252900     0.036831      13.81
 O      -2.596172     2.515278     0.130813     228.42
 C      -3.959251     2.821046    -0.347178     108.42
 H      -3.909485     2.464739    -1.448357      24.09
 H      -4.548680     2.526940     0.539304      24.74
 H      -4.079479     3.825573    -0.603552      26.69
 C      -0.626766     1.035788     0.137758      19.07
 O       0.131894     1.970208     0.761141     263.80
 C      -0.196198    -0.242328    -0.392736      53.70
 H       0.768177    -0.433768     0.006615      17.67
 C      -2.340704    -1.029724    -0.990413       9.47
 C      -3.345677    -2.387465    -1.425085      72.97
 H      -4.247195    -1.643575    -1.557348      22.30
 O      -3.137703    -2.950746    -2.685254     326.90
 H      -3.031155    -3.810757    -2.448686      26.33
 C      -3.653893    -3.427279    -0.291741      86.17
 H      -2.537033    -3.798252    -0.181709      19.05
 O      -4.390674    -2.874867     0.839199     311.97
 H      -3.797848    -2.605179     1.674986      22.83
 C      -4.539981    -4.632557    -0.592086      83.51
 O      -3.825070    -5.639570    -1.243900     313.18
 H      -3.110776    -5.773692    -0.477318      25.66
 H      -5.356329    -4.217805    -1.327087      24.52
 H      -4.916453    -5.164968     0.362269      24.35
55
name = lig-etoh-frame_71
 C       2.592443     1.734696    -1.840264      76.53
 H       2.438528     2.511446    -2.710622      24.86
 C       3.605066     1.106708     0.301466      74.69
 H       4.196973     1.446310     1.118079      24.04
 C       3.882669    -0.131322    -0.219419      -1.05
 O       4.603763    -1.374415     0.471173     211.17
 C       5.422115    -1.077616     1.580891     120.32
 H       4.731076    -0.483233     2.294339      24.18
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 H       6.326614    -0.731001     1.379796      28.96
 H       5.643330    -2.061783     2.162793      25.39
 C       3.623314    -0.440630    -1.593693      14.43
 O       4.042111    -1.698986    -2.172634     217.58
 H       4.368135    -2.067053    -1.372752      24.10
 C       3.301545     0.601358    -2.426951      35.29
 H       3.274393     0.448910    -3.447735      19.57
 C       2.921622     2.102153    -0.487841      15.75
 C       2.146499     3.343153     0.142566      99.26
 H       2.172065     4.414272    -0.408503      15.04
 O       2.586540     3.504282     1.457441     303.22
 H       3.533919     3.846952     1.330518      27.87
 C       0.601901     3.131937     0.051405      69.51
 H       0.419448     2.975667    -1.048764      19.25
 C      -0.102985     4.420627     0.431066      90.40
 O       0.508896     5.651466    -0.433286     144.03
 H       0.723342     5.548480    -1.427994      27.21
 H      -0.014107     4.832367     1.517742      22.50
 H      -1.010848     4.392774    -0.132173      22.85
 C      -0.976315    -1.258733    -0.906392      36.45
 H      -0.301814    -2.121708    -1.169791      17.08
 C      -2.790115     0.236903    -0.549745      45.57
 H      -3.791632     0.404189    -0.670334      17.37
 C      -2.014903     1.243039    -0.041507      17.25
 O      -2.657658     2.494915     0.138840     219.22
 C      -3.936007     2.823208    -0.383293      80.78
 H      -3.723612     2.466953    -1.370177      24.96
 H      -4.813120     2.324150     0.478056      20.26
 H      -3.887053     3.985835    -0.598963      23.51
 C      -0.651822     0.973965     0.161183      11.44
 O       0.137549     1.973998     0.785675     248.60
 C      -0.181669    -0.196379    -0.356634      55.83
 H       0.936621    -0.518409     0.017633      14.42
 C      -2.411789    -1.087872    -1.032838      20.71
 C      -3.438881    -2.274269    -1.334040      70.01
 H      -4.339735    -1.781016    -1.539573      24.37
 O      -3.112148    -2.952098    -2.697815     255.26
 H      -2.876985    -3.988239    -2.563717      20.32
 C      -3.593760    -3.450455    -0.259624      94.50
 H      -2.584408    -3.679511     0.012836      22.91
 O      -4.381835    -2.834167     0.839549     327.64
 H      -3.822612    -2.560672     1.603306      25.06
 C      -4.621872    -4.606123    -0.586203      89.15
 O      -3.799293    -5.711669    -1.249101     333.71
 H      -2.993277    -6.020150    -0.849066      30.81
 H      -5.349441    -4.243992    -1.253028      27.46
 H      -5.121558    -4.976437     0.283113      26.97
55
name = lig-etoh-frame_72
 C       2.646412     1.774549    -1.795908      88.93
 H       2.725556     2.390360    -2.650089      26.36
 C       3.662040     1.173070     0.276320      57.44
 H       4.140056     1.473730     1.242411      20.35
 C       3.848806    -0.227765    -0.219365       9.26
 O       4.570382    -1.305860     0.433781     213.02
 C       5.406552    -1.040501     1.612896     107.72
 H       4.805839    -0.626954     2.377409      26.21
 H       6.478061    -0.430992     1.325336      24.47
 H       5.444992    -2.082700     1.976060      25.25
 C       3.673061    -0.459066    -1.569849      15.20
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 O       4.088640    -1.690029    -2.162099     194.54
 H       4.259590    -2.342681    -1.366680      22.56
 C       3.266244     0.613296    -2.389147      35.46
 H       3.355427     0.638280    -3.547497      17.24
 C       2.922124     2.122657    -0.490760      39.58
 C       2.223618     3.303972     0.148264     118.30
 H       2.433244     4.195038    -0.393674      16.44
 O       2.584047     3.514600     1.447399     305.26
 H       3.587674     3.801546     1.550927      26.92
 C       0.609491     3.183724    -0.023932      42.33
 H       0.372007     2.841335    -1.024073      21.62
 C      -0.125294     4.541178     0.405739      95.59
 O       0.511004     5.651226    -0.445488     229.06
 H       0.802957     5.389355    -1.350898      27.33
 H      -0.128180     4.813710     1.490662      23.21
 H      -1.232264     4.366404     0.182357      22.62
 C      -1.041962    -1.239864    -0.939927      34.88
 H      -0.591559    -2.197462    -1.186632      20.63
 C      -2.864580     0.155551    -0.594197      44.84
 H      -4.025464     0.226178    -0.710610      16.33
 C      -2.006747     1.257642    -0.139297      16.07
 O      -2.656562     2.482206     0.189794     215.86
 C      -3.895559     2.826326    -0.437849     110.93
 H      -4.112392     2.282826    -1.489643      24.03
 H      -4.829190     2.442108     0.042671      25.21
 H      -3.874023     3.897293    -0.229528      24.80
 C      -0.681467     0.985615     0.187004       0.57
 O       0.146102     1.963075     0.827763     219.61
 C      -0.128406    -0.202639    -0.285729      46.44
 H       0.988260    -0.486131    -0.274508      14.93
 C      -2.433673    -1.153017    -1.037779      28.57
 C      -3.506846    -2.171642    -1.279690      56.70
 H      -4.660804    -1.957538    -1.483512      21.84
 O      -3.074604    -2.947171    -2.693837     216.10
 H      -2.895116    -3.962921    -2.598681      19.76
 C      -3.587178    -3.415188    -0.198567      72.80
 H      -2.626919    -3.805557     0.312008      20.39
 O      -4.364131    -2.784684     0.848104     294.26
 H      -3.729956    -2.423514     1.511117      23.34
 C      -4.604901    -4.606999    -0.600413      55.91
 O      -3.806912    -5.774588    -1.283794     242.83
 H      -2.937237    -6.167842    -0.849505      25.20
 H      -5.437160    -4.320753    -1.433336      25.18
 H      -5.279604    -4.774812     0.371990      25.54
55
name = lig-etoh-frame_73
 C       2.774342     1.787929    -1.830426      35.52
 H       2.557231     2.715628    -2.512035      20.03
 C       3.721611     1.189662     0.261688      58.55
 H       3.858400     1.411959     1.348526      16.14
 C       3.853526    -0.260398    -0.179311      25.13
 O       4.529258    -1.217554     0.394628     218.71
 C       5.387811    -1.013803     1.622415     111.57
 H       4.897963    -0.428282     2.509517      25.70
 H       6.157146    -0.425488     1.428813      30.12
 H       5.619696    -2.084880     1.825172      26.07
 C       3.723989    -0.508256    -1.592139       8.10
 O       4.127127    -1.667210    -2.138046     182.39
 H       4.157579    -2.584225    -1.527545      20.89
 C       3.198601     0.619722    -2.357291      55.57
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 H       3.407440     0.638941    -3.418856      25.14
 C       2.916210     2.104041    -0.458512      53.93
 C       2.273405     3.269314     0.108766     102.87
 H       2.787306     4.120864    -0.608866      20.16
 O       2.587141     3.533273     1.500289     314.24
 H       3.494143     3.788150     1.572701      32.27
 C       0.632702     3.216175    -0.049555      31.76
 H       0.337566     2.893196    -1.120785      18.53
 C      -0.147763     4.636437     0.318091     107.57
 O       0.489142     5.642224    -0.425226     243.69
 H       0.701575     5.049457    -1.332350      26.01
 H       0.005326     4.833990     1.425926      24.20
 H      -1.228560     4.484480     0.440932      24.08
 C      -1.047405    -1.228540    -0.938543      41.29
 H      -0.759283    -2.256347    -1.227518      20.64
 C      -2.959929     0.080274    -0.655829      35.10
 H      -4.036678     0.294174    -0.628081      18.04
 C      -2.101766     1.239085    -0.235662      -0.06
 O      -2.627246     2.449069     0.240984     204.36
 C      -3.844885     2.817538    -0.511476     115.88
 H      -4.229361     2.548111    -1.479180      26.53
 H      -4.987448     2.491812     0.102051      23.13
 H      -3.993678     3.888646    -0.222690      25.43
 C      -0.668034     1.041104     0.204172      -8.31
 O       0.150069     1.960839     0.864171     183.41
 C      -0.132515    -0.281091    -0.264452      26.99
 H       1.003227    -0.400561    -0.395970      14.99
 C      -2.463497    -1.140405    -1.001831      28.55
 C      -3.538349    -2.199752    -1.277491      73.89
 H      -4.535513    -1.927188    -1.346579      24.59
 O      -3.039305    -2.916228    -2.672992     248.02
 H      -3.061902    -3.804689    -2.432466      22.54
 C      -3.629468    -3.355499    -0.135439      84.14
 H      -2.770058    -3.895812     0.275196      20.25
 O      -4.348082    -2.725947     0.880794     330.84
 H      -3.643213    -2.190481     1.472051      21.69
 C      -4.545617    -4.619859    -0.642538      95.28
 O      -3.837972    -5.819724    -1.317469     276.16
 H      -3.222662    -6.008937    -0.545950      27.24
 H      -5.159404    -4.417023    -1.418130      29.24
 H      -5.042223    -4.824144     0.245662      28.78
55
name = lig-etoh-frame_74
 C       2.898619     1.871672    -1.872882      34.79
 H       2.290266     2.673666    -2.250329      19.04
 C       3.741002     1.137793     0.284586      65.45
 H       3.649368     1.294613     1.344421      17.65
 C       3.864445    -0.162989    -0.192867      23.19
 O       4.527033    -1.171576     0.420394     226.19
 C       5.312289    -0.999313     1.629550     108.21
 H       4.893208    -0.495109     2.440532      27.54
 H       6.275177    -0.252133     1.296897      24.81
 H       5.950111    -1.951534     1.813374      25.06
 C       3.727132    -0.498325    -1.582335      11.68
 O       4.164873    -1.678033    -2.146289     263.71
 H       4.086528    -2.365019    -1.613819      28.53
 C       3.168538     0.560987    -2.359562      60.85
 H       3.320092     0.470531    -3.452812      25.86
 C       2.940226     2.008610    -0.433980      63.81
 C       2.303224     3.296122     0.067309     106.32
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 H       2.699674     4.037775    -0.534545      25.64
 O       2.566833     3.550309     1.553411     286.17
 H       3.598789     3.875772     1.496625      28.60
 C       0.647865     3.238537    -0.050252      38.37
 H       0.412887     3.040540    -1.057295      19.70
 C      -0.140983     4.655489     0.304842     114.54
 O       0.455547     5.614047    -0.441736     268.31
 H       0.584247     5.331502    -1.308181      34.04
 H       0.375627     4.846610     1.312823      24.12
 H      -1.262170     4.649186     0.225247      24.86
 C      -1.024283    -1.247267    -0.903306      48.68
 H      -0.624053    -2.219808    -1.261380      21.15
 C      -3.040062     0.118487    -0.686591      40.25
 H      -4.088063     0.365459    -0.622487      19.23
 C      -2.161304     1.178366    -0.269033      -7.75
 O      -2.627072     2.403640     0.243345     201.15
 C      -3.852040     2.847378    -0.504408     101.37
 H      -3.852727     2.732409    -1.684158      24.58
 H      -4.690738     2.463341     0.270487      22.37
 H      -4.001327     3.984701    -0.492885      25.35
 C      -0.682111     1.040140     0.160952      -8.88
 O       0.147760     1.981447     0.871808     158.23
 C      -0.200692    -0.341062    -0.272391      25.01
 H       1.009269    -0.335489    -0.395016      14.40
 C      -2.500200    -1.114405    -0.957525      18.31
 C      -3.472567    -2.311785    -1.302785      63.52
 H      -4.514129    -1.694843    -1.368126      22.20
 O      -3.018044    -2.857497    -2.618635     239.29
 H      -3.283106    -3.867261    -2.304190      19.25
 C      -3.687568    -3.322027    -0.130575      80.48
 H      -2.672381    -3.776687     0.128207      20.12
 O      -4.336628    -2.651244     0.943993     365.93
 H      -3.722910    -2.145608     1.443401      27.76
 C      -4.453472    -4.628247    -0.701686      79.92
 O      -3.865708    -5.827826    -1.304363     269.25
 H      -3.400097    -6.102782    -0.493697      27.97
 H      -5.239204    -4.244674    -1.556290      24.94
 H      -4.953518    -5.139928     0.274009      24.01
55
name = lig-etoh-frame_75
 C       2.985105     1.926768    -1.855076      37.52
 H       2.182602     2.513004    -2.399528      17.54
 C       3.700799     1.078649     0.359436      62.22
 H       3.636407     1.176663     1.483954      16.23
 C       3.923263    -0.078941    -0.247974      10.90
 O       4.537482    -1.172623     0.486431     246.50
 C       5.322324    -0.947569     1.589665     124.78
 H       4.674390    -0.634185     2.534681      25.37
 H       6.002830    -0.268929     1.305623      29.56
 H       5.891625    -1.791965     1.872379      27.15
 C       3.692743    -0.436068    -1.563824      11.21
 O       4.195817    -1.672239    -2.180232     191.64
 H       4.041502    -2.374466    -1.378562      22.39
 C       3.177619     0.507999    -2.412252      61.29
 H       3.018533     0.193920    -3.511363      24.03
 C       2.977068     1.950388    -0.465486      69.62
 C       2.278128     3.300906     0.100797      94.82
 H       2.569722     4.325017    -0.529094      23.50
 O       2.561480     3.575452     1.563625     295.34
 H       3.474829     3.899124     1.588380      31.42
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 C       0.656556     3.249110    -0.022826      48.94
 H       0.435953     3.020445    -1.152577      16.86
 C      -0.087245     4.588678     0.353026     109.78
 O       0.437976     5.634729    -0.495680     212.98
 H       0.482693     5.617048    -1.572471      26.82
 H       0.285157     4.841599     1.330940      25.43
 H      -1.147540     4.630526     0.082648      24.22
 C      -1.049883    -1.302525    -0.861430      46.82
 H      -0.459686    -2.126750    -1.233605      21.99
 C      -3.080668     0.204205    -0.693578      45.53
 H      -4.251156     0.368168    -0.730153      22.54
 C      -2.141366     1.144937    -0.216957       7.82
 O      -2.646240     2.373240     0.202595     218.53
 C      -3.851653     2.923046    -0.501594      87.89
 H      -3.499258     2.601023    -1.441109      26.47
 H      -4.627458     2.265101     0.240726      20.55
 H      -3.837552     4.002289    -0.513784      25.64
 C      -0.743721     0.967244     0.069641      13.01
 O       0.129142     2.010438     0.829661     149.60
 C      -0.245466    -0.299615    -0.274664      31.72
 H       0.801592    -0.472451    -0.269405      16.26
 C      -2.500737    -1.127909    -0.923785      13.86
 C      -3.405101    -2.339266    -1.326415      84.86
 H      -4.270492    -1.802244    -1.541838      22.46
 O      -3.016985    -2.833952    -2.523410     310.10
 H      -3.277130    -3.767451    -2.725997      23.59
 C      -3.689869    -3.326055    -0.166940      84.03
 H      -2.624775    -3.492298     0.093335      21.29
 O      -4.348110    -2.597677     0.990967     327.72
 H      -3.577584    -2.141417     1.566209      20.16
 C      -4.446533    -4.631169    -0.730633     123.80
 O      -3.868474    -5.810111    -1.279261     313.89
 H      -3.322266    -6.440823    -0.663718      26.46
 H      -5.192014    -4.227123    -1.283643      29.02
 H      -4.968320    -5.042228     0.038049      26.37
55
name = lig-etoh-frame_76
 C       3.015346     1.871149    -1.874325      47.00
 H       2.381594     2.411537    -2.589483      19.66
 C       3.603957     1.065918     0.460916      38.62
 H       3.739656     1.131199     1.500472      18.16
 C       4.053351    -0.108402    -0.252653      -1.67
 O       4.516173    -1.199257     0.509123     242.18
 C       5.324774    -0.872173     1.602899     100.98
 H       4.663346    -0.755231     2.423943      26.09
 H       6.042557     0.119158     1.410622      25.85
 H       5.816223    -1.911061     1.917769      23.76
 C       3.679683    -0.407647    -1.607872      21.79
 O       4.197291    -1.654872    -2.178571     190.45
 H       4.184360    -2.298288    -1.310597      23.97
 C       3.181894     0.526200    -2.483430      69.85
 H       2.780544     0.133393    -3.378978      20.34
 C       3.005384     2.018272    -0.481957      44.68
 C       2.229508     3.316222     0.162939     113.90
 H       2.426492     4.157173    -0.344064      24.56
 O       2.541164     3.593620     1.546378     300.33
 H       3.497735     3.939002     1.643446      28.23
 C       0.663307     3.211163    -0.009610      76.24
 H       0.470843     3.013857    -1.003147      17.92
 C      -0.004909     4.500583     0.358931      95.94
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 O       0.442124     5.692127    -0.555914     194.07
 H       0.234929     5.494898    -1.581654      26.51
 H      -0.056704     4.912694     1.480940      22.90
 H      -1.099367     4.323451     0.235110      22.22
 C      -1.113022    -1.337739    -0.806119      52.73
 H      -0.493660    -2.211530    -1.150075      18.49
 C      -3.072271     0.215026    -0.698474      65.18
 H      -4.063025     0.358214    -0.827853      26.49
 C      -2.150606     1.168400    -0.132645       3.68
 O      -2.643030     2.380160     0.174779     196.16
 C      -3.803101     2.940125    -0.481675      80.50
 H      -3.678487     2.426816    -1.532984      24.61
 H      -4.848258     2.421503    -0.087914      22.45
 H      -3.714035     4.115821    -0.285038      22.66
 C      -0.791186     0.925039    -0.000821      21.38
 O       0.086670     2.026445     0.742413     164.52
 C      -0.280473    -0.242352    -0.291843      47.01
 H       0.855114    -0.690360     0.007647      14.57
 C      -2.479187    -1.140552    -0.906040      26.05
 C      -3.389378    -2.280492    -1.301548      62.51
 H      -4.488165    -1.841619    -1.637887      20.43
 O      -2.975499    -2.853138    -2.495841     319.59
 H      -3.272918    -3.607729    -2.942300      24.45
 C      -3.634485    -3.324801    -0.196630      86.55
 H      -2.646572    -3.540997     0.251568      20.16
 O      -4.349561    -2.564937     1.007558     279.02
 H      -3.552320    -2.371076     1.577525      22.41
 C      -4.454327    -4.624909    -0.679144      78.73
 O      -3.849256    -5.795224    -1.291422     294.66
 H      -3.255128    -6.359242    -0.752094      27.88
 H      -5.324379    -4.236634    -1.457707      25.55
 H      -5.213083    -4.846157     0.267659      24.28
55
name = lig-etoh-frame_77
 C       2.993542     1.759886    -1.932208      67.96
 H       2.642266     2.596997    -2.591598      24.82
 C       3.503280     1.048451     0.461186      38.81
 H       3.761847     1.238445     1.562143      20.05
 C       4.145715    -0.136258    -0.217821       4.97
 O       4.495582    -1.234330     0.490695     233.06
 C       5.351615    -0.815603     1.651824     112.15
 H       4.630339    -0.605248     2.527834      24.86
 H       5.896092     0.060395     1.607578      29.37
 H       5.886557    -1.668295     1.802942      27.12
 C       3.734473    -0.431361    -1.657629      14.47
 O       4.175119    -1.628666    -2.145242     236.31
 H       4.387738    -2.179725    -1.492820      28.52
 C       3.190393     0.581249    -2.507778      47.59
 H       2.578155     0.267329    -3.461605      19.19
 C       3.030432     2.137268    -0.435928      16.09
 C       2.186812     3.283945     0.221693     100.08
 H       2.456828     4.275486    -0.494368      18.19
 O       2.516470     3.604869     1.540998     278.04
 H       3.509581     3.943439     1.498727      25.91
 C       0.694521     3.129429     0.017300      67.91
 H       0.509515     3.026811    -1.146130      14.84
 C       0.017839     4.469860     0.355248      95.31
 O       0.421771     5.712497    -0.588124     201.93
 H       0.214833     5.299556    -1.399188      30.27
 H      -0.020340     4.838335     1.304206      25.23
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 H      -1.011886     4.073943     0.268828      21.83
 C      -1.134688    -1.341136    -0.737708      44.72
 H      -0.798958    -2.344343    -0.933971      17.80
 C      -2.971208     0.158769    -0.681337      55.62
 H      -4.133243     0.412946    -0.924202      23.28
 C      -2.236392     1.184021    -0.087787      19.94
 O      -2.633481     2.431588     0.179196     250.04
 C      -3.744023     2.909061    -0.477941     136.75
 H      -4.005521     2.774535    -1.561062      26.67
 H      -4.936725     2.931612    -0.324589      24.28
 H      -3.693243     3.905314    -0.270544      28.26
 C      -0.792529     1.006010    -0.008318      24.00
 O       0.022926     2.016317     0.641667     230.00
 C      -0.261775    -0.315250    -0.316181      36.38
 H       0.616756    -0.472060     0.077104      17.17
 C      -2.491646    -1.117807    -0.908249      31.10
 C      -3.470261    -2.209191    -1.277825      78.58
 H      -4.451767    -1.907630    -1.382639      24.39
 O      -2.870709    -2.871818    -2.518054     194.26
 H      -3.582588    -3.623227    -2.928827      20.59
 C      -3.577105    -3.315868    -0.184634      77.67
 H      -2.703156    -3.819287     0.333658      18.50
 O      -4.334519    -2.570421     0.979951     305.26
 H      -3.627932    -2.448263     1.630015      25.21
 C      -4.526516    -4.594270    -0.595355      96.86
 O      -3.834567    -5.763250    -1.313263     280.27
 H      -3.149071    -6.032937    -0.617195      26.71
 H      -5.043117    -4.389804    -1.448828      29.67
 H      -5.047693    -4.731862     0.259210      28.88
55
name = lig-etoh-frame_78
 C       2.923020     1.782708    -1.910015      81.88
 H       2.881826     2.732191    -2.485688      26.79
 C       3.448460     1.041204     0.384713      47.52
 H       3.574114     1.319281     1.406502      21.92
 C       4.122074    -0.104322    -0.236329      14.46
 O       4.514886    -1.264841     0.492405     218.18
 C       5.321405    -0.795985     1.720501      89.91
 H       4.696104    -0.557687     2.579345      24.80
 H       5.961506     0.195684     1.483625      25.12
 H       6.227758    -1.592138     1.858638      23.44
 C       3.833781    -0.436074    -1.637500       9.65
 O       4.136752    -1.610912    -2.145192     153.74
 H       4.732954    -2.223283    -1.408399      20.29
 C       3.196664     0.551426    -2.527232      42.36
 H       2.774451     0.510215    -3.471775      21.10
 C       3.063091     2.167603    -0.393687      15.92
 C       2.195085     3.265927     0.194664     116.48
 H       2.323308     4.062007    -0.398735      22.57
 O       2.509640     3.618238     1.555822     324.01
 H       3.391987     3.909613     1.444118      30.36
 C       0.723175     3.061917    -0.018435      61.78
 H       0.666077     3.034897    -1.058848      17.69
 C      -0.005966     4.464061     0.320081      80.10
 O       0.368921     5.674027    -0.570757     156.62
 H       0.383322     5.136326    -1.592370      22.99
 H       0.328928     4.837528     1.432696      21.19
 H      -1.060527     4.201896     0.103447      20.69
 C      -1.132819    -1.363338    -0.670430      40.92
 H      -0.974087    -2.476495    -0.637047      16.12
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 C      -2.941355     0.138573    -0.657547      62.66
 H      -3.888917     0.347845    -0.890986      23.07
 C      -2.242220     1.174154    -0.074973      13.96
 O      -2.643683     2.485963     0.200445     233.76
 C      -3.762222     2.952139    -0.523326     105.98
 H      -3.756073     3.018505    -1.632229      25.46
 H      -4.934533     2.894649     0.061681      21.80
 H      -3.581562     4.160152    -0.380697      23.79
 C      -0.795088     1.074994    -0.006313      27.73
 O      -0.045607     1.984433     0.561109     230.13
 C      -0.279354    -0.351442    -0.320822      27.32
 H       0.911170    -0.360649     0.130589      13.71
 C      -2.522072    -1.097347    -0.923340      29.96
 C      -3.494972    -2.201300    -1.257678      51.33
 H      -4.635201    -1.781367    -1.300742      22.13
 O      -2.796916    -2.892918    -2.545256     212.06
 H      -3.582672    -3.391952    -2.676480      23.61
 C      -3.568871    -3.327003    -0.130274      85.04
 H      -2.672779    -3.846390     0.180756      19.64
 O      -4.304992    -2.607954     0.918865     301.33
 H      -3.685048    -2.345643     1.737852      23.29
 C      -4.542339    -4.542531    -0.560214      64.50
 O      -3.815875    -5.712930    -1.286018     290.36
 H      -2.998392    -5.798159    -0.658358      25.14
 H      -5.232952    -4.234105    -1.482146      25.79
 H      -5.082962    -4.921028     0.476694      24.81
55
name = lig-etoh-frame_79
 C       2.875038     1.886535    -1.818144     120.93
 H       2.819807     2.709432    -2.522556      25.23
 C       3.444787     1.046296     0.290440      30.29
 H       3.366254     1.190137     1.401412      19.53
 C       4.027555    -0.077855    -0.276372      11.82
 O       4.563089    -1.265414     0.526741     212.28
 C       5.341544    -0.785519     1.750792     111.61
 H       4.704560    -0.639574     2.637509      25.78
 H       5.736267     0.094274     1.259172      25.56
 H       6.117932    -1.395021     2.012224      27.22
 C       3.907049    -0.375687    -1.603014      28.30
 O       4.123313    -1.653627    -2.147961     209.68
 H       4.864395    -1.980249    -1.567216      23.77
 C       3.216513     0.532811    -2.474516      44.10
 H       3.163438     0.499255    -3.668043      20.77
 C       3.071287     2.100449    -0.429811      31.01
 C       2.226898     3.220900     0.168534      79.72
 H       2.303591     4.266487    -0.517587      19.59
 O       2.502092     3.625696     1.572734     263.79
 H       3.521935     3.988404     1.584406      24.75
 C       0.712466     3.048178    -0.083403      39.71
 H       0.703722     2.887126    -1.235110      15.61
 C      -0.023369     4.474309     0.291789     108.48
 O       0.307717     5.568978    -0.569716     279.85
 H       0.627726     5.435842    -1.411444      32.82
 H       0.390358     4.668232     1.192349      25.34
 H      -1.111083     4.493895     0.179333      22.98
 C      -1.149415    -1.424558    -0.606957      36.84
 H      -0.819744    -2.437208    -0.390481      16.13
 C      -2.976781     0.179075    -0.628045      58.85
 H      -4.131695     0.385395    -0.886721      18.49
 C      -2.156500     1.201719    -0.077907       4.86
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 O      -2.666287     2.518317     0.219291     242.56
 C      -3.831076     3.120630    -0.553411      98.24
 H      -3.505447     2.823123    -1.600270      25.15
 H      -4.393851     2.571384     0.201380      21.01
 H      -3.639085     4.104235    -0.466452      27.77
 C      -0.833352     1.011876    -0.045014      41.03
 O      -0.071273     1.980505     0.527938     244.40
 C      -0.257859    -0.294561    -0.262327      35.38
 H       0.703424    -0.499025    -0.174995      16.98
 C      -2.512579    -1.126015    -0.929759      37.59
 C      -3.465249    -2.223592    -1.241110      62.30
 H      -4.413339    -1.815082    -1.490039      26.43
 O      -2.774228    -2.886166    -2.532404     224.40
 H      -3.496825    -3.503904    -2.770714      24.00
 C      -3.614759    -3.341368    -0.093044      77.47
 H      -2.512859    -3.660952     0.049199      20.05
 O      -4.268481    -2.654667     0.878463     359.15
 H      -3.704814    -2.251766     1.527358      28.83
 C      -4.546969    -4.510619    -0.554988      99.29
 O      -3.800065    -5.622374    -1.223685     397.60
 H      -2.948665    -5.863910    -0.848589      32.01
 H      -5.429297    -4.089081    -1.010649      28.63
 H      -4.986249    -5.000322     0.224152      26.58
55
name = lig-etoh-frame_80
 C       2.882215     1.926440    -1.804141      91.24
 H       2.499245     2.682555    -2.554581      23.42
 C       3.485366     1.021596     0.286164      47.57
 H       3.222065     0.921447     1.341480      17.07
 C       3.950625    -0.128785    -0.250698      -6.82
 O       4.605324    -1.237729     0.563849     212.73
 C       5.335103    -0.758192     1.727144      89.88
 H       4.623026    -0.627540     2.631049      24.49
 H       5.696088     0.256509     1.380182      24.41
 H       6.165539    -1.545469     2.109328      23.70
 C       3.920545    -0.329120    -1.651926      15.79
 O       4.133787    -1.686455    -2.143632     229.03
 H       4.920423    -1.984893    -1.705380      24.53
 C       3.247149     0.615044    -2.391911      76.27
 H       3.558788     0.363586    -3.363003      25.83
 C       3.009927     2.072258    -0.512317      44.15
 C       2.262541     3.235291     0.142212     110.29
 H       2.466912     4.049598    -0.397093      25.25
 O       2.511753     3.625895     1.574312     326.83
 H       3.408347     3.954227     1.703192      30.49
 C       0.649523     3.062860    -0.190836      54.02
 H       0.607835     2.768682    -1.226380      17.63
 C      -0.038626     4.440771     0.219032      99.89
 O       0.260124     5.503931    -0.560620     273.90
 H       0.829840     5.417362    -1.418799      27.99
 H       0.387560     4.642870     1.354073      22.77
 H      -1.148454     4.463545     0.502480      23.57
 C      -1.145891    -1.432036    -0.529139      54.63
 H      -0.606539    -2.382346    -0.363532      15.16
 C      -3.052962     0.225331    -0.615020      52.19
 H      -4.081507     0.410700    -0.744918      19.20
 C      -2.180130     1.270138    -0.125176      -3.34
 O      -2.642675     2.537653     0.246709     193.35
 C      -3.827967     3.212428    -0.574648      74.27
 H      -3.763305     2.623718    -1.493275      25.77
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 H      -4.634453     2.531870    -0.025276      21.63
 H      -3.813323     4.446228    -0.424741      22.51
 C      -0.793811     0.914439    -0.079234      43.50
 O      -0.052197     2.001878     0.534412     233.55
 C      -0.302922    -0.281639    -0.220270      50.64
 H       0.869778    -0.609645    -0.343773      13.64
 C      -2.479672    -1.147576    -0.890150      30.14
 C      -3.385380    -2.289112    -1.274335      54.47
 H      -4.393097    -1.860881    -1.735153      22.45
 O      -2.794693    -2.864432    -2.488805     238.52
 H      -3.174523    -3.756610    -3.003509      21.79
 C      -3.629984    -3.348365    -0.137677      89.17
 H      -2.625387    -3.565383     0.125039      24.23
 O      -4.261899    -2.685918     0.891649     359.79
 H      -3.537153    -2.146585     1.348348      24.48
 C      -4.501894    -4.507840    -0.532001      83.24
 O      -3.814466    -5.510775    -1.197845     376.34
 H      -2.956518    -5.868885    -0.759755      28.63
 H      -5.501882    -4.061688    -0.925859      25.44
 H      -4.963815    -5.079623     0.450253      23.37
55
name = lig-etoh-frame_81
 C       2.899796     1.914299    -1.933022      40.99
 H       2.252745     2.587761    -2.431495      20.34
 C       3.514166     0.989929     0.335220      59.27
 H       3.212395     0.908004     1.371740      16.77
 C       3.934571    -0.253488    -0.201798      -2.13
 O       4.627877    -1.190881     0.574819     236.28
 C       5.322247    -0.719505     1.708021     113.36
 H       4.615312    -0.587488     2.496120      27.16
 H       5.835561     0.303216     1.811526      25.76
 H       5.998210    -1.486831     1.917204      27.19
 C       3.904507    -0.357713    -1.666097      19.61
 O       4.141044    -1.678117    -2.145883     165.98
 H       5.110919    -2.120362    -1.771672      20.43
 C       3.320139     0.725179    -2.328507      73.90
 H       3.581722     0.458390    -3.420299      26.72
 C       2.920803     2.073569    -0.488455      63.56
 C       2.270202     3.252168     0.139179      95.58
 H       2.749217     4.206306    -0.521197      23.52
 O       2.498370     3.600146     1.557264     296.47
 H       3.467777     3.924543     1.603217      29.15
 C       0.574979     3.084057    -0.267114      62.51
 H       0.469280     2.832732    -1.353825      17.00
 C      -0.054053     4.356883     0.231424     112.64
 O       0.227727     5.512037    -0.582419     266.12
 H       0.816921     5.039506    -1.337397      28.57
 H       0.342746     4.554793     1.151992      27.19
 H      -1.070024     4.176720     0.509647      25.74
 C      -1.130041    -1.395053    -0.450185      45.84
 H      -0.622836    -2.380891    -0.578439      14.22
 C      -3.070883     0.237755    -0.605675      40.75
 H      -4.211253     0.406974    -0.674243      20.59
 C      -2.269054     1.307468    -0.208568       0.19
 O      -2.608670     2.572096     0.264219     195.77
 C      -3.815816     3.215948    -0.539941     114.31
 H      -3.977490     2.842516    -1.611132      25.88
 H      -4.981436     3.125881    -0.392907      25.05
 H      -3.920202     4.201222    -0.496411      28.55
 C      -0.758127     0.965182    -0.064213      46.66
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 O      -0.008057     2.013510     0.553478     214.67
 C      -0.296321    -0.394661    -0.210936      24.81
 H       0.775078    -0.383962    -0.254700      15.86
 C      -2.465667    -1.136680    -0.808948      40.13
 C      -3.351686    -2.362290    -1.359667      80.03
 H      -4.327285    -1.942367    -1.638420      24.12
 O      -2.789037    -2.859387    -2.478244     318.49
 H      -2.938660    -3.731952    -2.724823      26.07
 C      -3.616967    -3.330525    -0.216968      84.01
 H      -2.648752    -3.785705     0.279972      19.53
 O      -4.268103    -2.687519     0.954404     322.74
 H      -3.483220    -2.059500     1.214050      22.46
 C      -4.493645    -4.528589    -0.430466     101.69
 O      -3.819376    -5.425691    -1.227111     379.15
 H      -3.186693    -5.744187    -0.521498      28.71
 H      -5.292161    -4.277766    -1.145161      27.73
 H      -4.743209    -4.790765     0.544648      28.80
55
name = lig-etoh-frame_82
 C       2.890150     1.944900    -1.967942      23.88
 H       2.152437     2.557239    -2.574869      15.73
 C       3.494469     0.976579     0.367721      49.19
 H       3.368362     1.144857     1.490150      15.09
 C       3.941967    -0.328274    -0.188387      14.57
 O       4.644738    -1.146082     0.551340     232.70
 C       5.305504    -0.662999     1.732439      99.31
 H       4.496274    -0.666266     2.596371      24.10
 H       5.901576     0.219508     1.750150      26.74
 H       6.033692    -1.564334     1.885464      24.41
 C       3.883991    -0.431722    -1.572795      30.61
 O       4.162839    -1.657647    -2.169815     255.23
 H       4.964934    -1.994010    -1.862868      26.29
 C       3.459676     0.726954    -2.398176      54.43
 H       3.237628     0.753763    -3.483906      25.72
 C       2.867206     2.017835    -0.428460      58.89
 C       2.257425     3.306908     0.096586     107.46
 H       2.668666     4.066707    -0.405110      31.12
 O       2.477476     3.558820     1.519835     290.81
 H       3.477145     3.869294     1.419196      28.79
 C       0.547474     3.100996    -0.299520      73.95
 H       0.327520     2.986289    -1.400438      19.71
 C      -0.086749     4.282836     0.268361      97.75
 O       0.204116     5.511825    -0.619955     250.66
 H       0.537649     5.073663    -1.333992      37.07
 H       0.492180     4.493497     1.290313      25.03
 H      -1.195998     3.991938     0.240558      22.33
 C      -1.151849    -1.418859    -0.421982      29.72
 H      -0.854949    -2.391331    -0.779095      13.59
 C      -3.078513     0.201479    -0.607928      43.37
 H      -4.195663     0.290667    -0.675053      19.78
 C      -2.267299     1.307064    -0.268504       5.60
 O      -2.636225     2.619780     0.241533     183.76
 C      -3.841344     3.175886    -0.530564     111.39
 H      -3.708716     3.159629    -1.624008      25.48
 H      -4.945666     3.301704    -0.178495      24.63
 H      -3.579868     4.425175    -0.504054      24.37
 C      -0.795627     1.053212    -0.031852      24.99
 O       0.050462     2.003285     0.562130     208.02
 C      -0.242389    -0.372169    -0.176919      20.69
 H       0.893901    -0.403981    -0.046045      14.84
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 C      -2.502292    -1.106794    -0.723441      19.20
 C      -3.348709    -2.368996    -1.373151      70.64
 H      -4.449320    -1.920006    -1.513076      22.50
 O      -2.736692    -2.865604    -2.517747     257.33
 H      -2.898075    -3.919480    -2.358187      17.18
 C      -3.584575    -3.323971    -0.220866      97.69
 H      -2.751398    -3.864045     0.128919      21.64
 O      -4.253177    -2.663767     1.001927     303.63
 H      -3.657647    -2.023355     1.344311      27.37
 C      -4.524304    -4.495394    -0.372765      81.88
 O      -3.786268    -5.397976    -1.256515     327.72
 H      -3.209905    -5.897381    -0.634689      27.87
 H      -5.374581    -4.355380    -1.084382      26.88
 H      -4.756935    -4.771476     0.767830      25.68
55
name = lig-etoh-frame_83
 C       2.881658     1.933865    -1.881153      55.51
 H       2.400750     2.474927    -2.682702      22.87
 C       3.435950     0.983029     0.380963      50.47
 H       3.657077     1.297258     1.371632      19.89
 C       3.920953    -0.254444    -0.176423      19.18
 O       4.686068    -1.144444     0.536155     236.75
 C       5.282194    -0.665924     1.800062     108.17
 H       4.615691    -0.651904     2.569859      27.21
 H       5.867717     0.298196     1.406625      25.11
 H       6.005392    -1.464895     2.028162      25.72
 C       3.847872    -0.477737    -1.526838      14.53
 O       4.173769    -1.630602    -2.215403     210.92
 H       5.043429    -1.986315    -1.820691      25.82
 C       3.565569     0.706986    -2.499791      18.97
 H       3.162472     0.626793    -3.518188      18.05
 C       2.846671     1.947303    -0.420559      16.70
 C       2.191714     3.289500     0.048930      87.70
 H       2.595584     4.286095    -0.572730      22.35
 O       2.462760     3.517762     1.462243     316.13
 H       3.343996     3.844341     1.504278      28.88
 C       0.589180     3.113656    -0.287300      75.85
 H       0.301604     2.973156    -1.307827      19.91
 C      -0.136944     4.276531     0.305779     110.93
 O       0.170132     5.493751    -0.624200     193.39
 H       0.283260     5.215646    -1.716057      25.38
 H       0.224500     4.436388     1.286412      26.10
 H      -1.165372     4.157258     0.180349      24.22
 C      -1.178846    -1.423727    -0.435449      22.21
 H      -0.952183    -2.475319    -0.804963      13.67
 C      -3.078819     0.157005    -0.607643      43.24
 H      -4.145487     0.250028    -0.760633      20.02
 C      -2.188772     1.307372    -0.273419      11.50
 O      -2.714350     2.636140     0.177249     206.13
 C      -3.820642     3.255317    -0.532680     117.41
 H      -3.532422     3.103021    -1.583125      24.30
 H      -4.681255     3.009090     0.245643      22.41
 H      -3.317680     4.109823    -0.369492      25.95
 C      -0.849186     1.071393    -0.002917      20.63
 O       0.110319     1.981412     0.550852     198.21
 C      -0.212334    -0.246504    -0.128983      46.54
 H       0.849290    -0.595197     0.222985      15.80
 C      -2.560010    -1.102533    -0.670689      13.04
 C      -3.377606    -2.274119    -1.306301      69.44
 H      -4.394154    -1.956612    -1.589311      22.70
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 O      -2.692187    -2.914852    -2.560558     228.56
 H      -2.731988    -3.866433    -2.142054      17.60
 C      -3.586078    -3.320004    -0.147662      88.28
 H      -2.527272    -3.798958     0.029938      19.50
 O      -4.228262    -2.638633     1.017962     292.61
 H      -3.661022    -1.968632     1.567704      24.39
 C      -4.570113    -4.456585    -0.351667      85.73
 O      -3.740014    -5.403998    -1.271441     330.95
 H      -3.112045    -6.128309    -0.919825      30.58
 H      -5.641076    -4.237197    -0.688948      26.42
 H      -4.801465    -4.976057     0.559227      27.09
55
name = lig-etoh-frame_84
 C       2.933836     1.796972    -1.804033      65.17
 H       2.661250     2.615314    -2.533160      24.90
 C       3.384786     0.989781     0.386873      65.43
 H       3.886527     1.343888     1.340305      20.21
 C       3.907579    -0.135459    -0.140853       0.47
 O       4.727742    -1.170286     0.540870     217.66
 C       5.293745    -0.670185     1.806237     109.39
 H       4.516911    -0.408107     2.720430      24.13
 H       5.672806     0.236450     1.510315      28.50
 H       6.067662    -1.387960     2.189664      25.37
 C       3.797934    -0.443836    -1.614247      -2.91
 O       4.197354    -1.613492    -2.254759     156.74
 H       5.051490    -2.098291    -1.726331      22.60
 C       3.583401     0.695006    -2.502903      37.04
 H       3.429595     0.252259    -3.563182      18.99
 C       2.815165     1.951956    -0.484231      39.89
 C       2.128027     3.252294    -0.016019     105.57
 H       2.357546     4.074653    -0.582443      23.39
 O       2.425558     3.477004     1.401691     299.54
 H       3.364325     3.922800     1.586950      27.06
 C       0.650522     3.121481    -0.211838      69.08
 H       0.425625     2.869012    -1.328984      19.21
 C      -0.187024     4.328430     0.266667     101.56
 O       0.143988     5.470964    -0.624237     257.16
 H      -0.087504     5.320464    -1.557064      29.81
 H      -0.018169     4.580208     1.405174      24.00
 H      -1.330681     4.261404     0.300926      23.39
 C      -1.173293    -1.347587    -0.460314      49.53
 H      -0.794179    -2.341257    -0.578142      17.08
 C      -3.052223     0.183079    -0.588255      40.70
 H      -4.171711     0.399961    -0.927144      20.02
 C      -2.181953     1.316606    -0.248593      31.52
 O      -2.745852     2.573983     0.108646     240.40
 C      -3.750437     3.317856    -0.506668     102.40
 H      -3.928041     2.901758    -1.587019      24.71
 H      -4.591840     2.908555     0.083097      24.53
 H      -3.425424     4.499997    -0.230273      22.89
 C      -0.813140     1.048636     0.039451      18.37
 O       0.158373     1.953997     0.533324     214.92
 C      -0.282854    -0.209176    -0.084829      54.37
 H       0.645240    -0.444173     0.311936      17.16
 C      -2.577651    -1.145348    -0.667174      52.33
 C      -3.404987    -2.183173    -1.229151      36.96
 H      -4.389364    -1.867525    -1.753971      22.33
 O      -2.673983    -2.959370    -2.538866     210.99
 H      -2.570752    -3.858668    -2.314035      21.83
 C      -3.589070    -3.298380    -0.040276     103.13
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 H      -2.585631    -3.592404     0.102566      23.50
 O      -4.199873    -2.609379     1.027603     331.48
 H      -3.472052    -2.150919     1.578738      21.94
 C      -4.577750    -4.477471    -0.348029      85.02
 O      -3.721347    -5.400807    -1.309157     331.09
 H      -3.203215    -6.095700    -0.817309      29.15
 H      -5.569551    -4.107035    -0.595256      27.54
 H      -4.722514    -5.195796     0.544398      25.99
55
name = lig-etoh-frame_85
 C       3.002298     1.671634    -1.852366      57.51
 H       2.858566     2.681016    -2.225243      21.03
 C       3.365209     1.029331     0.423260      58.49
 H       3.759294     1.347055     1.356687      23.28
 C       3.930694    -0.116765    -0.165555     -12.25
 O       4.745469    -1.177276     0.553752     208.45
 C       5.278379    -0.668544     1.818221     111.57
 H       4.565920    -0.389546     2.481158      28.07
 H       5.782378     0.434259     1.742333      26.98
 H       6.109125    -1.314756     2.290997      25.26
 C       3.786084    -0.377162    -1.692461      14.90
 O       4.235214    -1.608483    -2.273314     227.40
 H       4.755272    -2.049802    -1.725986      28.39
 C       3.546989     0.614026    -2.457977      69.49
 H       3.788529     0.348717    -3.456031      20.86
 C       2.782720     1.986228    -0.520727      46.68
 C       2.093576     3.188418    -0.036656     106.95
 H       2.366360     4.133299    -0.779452      21.49
 O       2.388209     3.447930     1.353935     314.51
 H       3.257626     3.917155     1.381737      29.65
 C       0.631806     3.106093    -0.141304      78.44
 H       0.604859     2.935463    -1.175935      19.51
 C      -0.251186     4.409362     0.218590     113.66
 O       0.116225     5.467690    -0.591802     298.42
 H      -0.306375     5.229334    -1.427090      30.51
 H      -0.040710     4.800217     1.223829      24.64
 H      -1.286742     4.101057     0.255804      23.64
 C      -1.154469    -1.239834    -0.469207      61.69
 H      -0.557886    -2.193560    -0.323467      18.14
 C      -3.023620     0.253555    -0.580275      41.12
 H      -3.947850     0.521611    -0.919799      21.29
 C      -2.230524     1.309756    -0.217192      15.44
 O      -2.709923     2.488620     0.058242     273.37
 C      -3.700362     3.368725    -0.488150     143.46
 H      -4.210333     3.111330    -1.427824      26.72
 H      -4.849994     3.138290    -0.139004      24.82
 H      -3.857616     4.371071    -0.433756      28.45
 C      -0.756056     1.067805     0.080836      19.56
 O       0.196663     1.922335     0.535559     218.07
 C      -0.418244    -0.265889    -0.052691      36.15
 H       0.747709    -0.258391     0.355350      14.33
 C      -2.535903    -1.132204    -0.697205      52.62
 C      -3.438408    -2.202822    -1.186907      39.02
 H      -4.304187    -1.744896    -1.793787      21.50
 O      -2.674371    -2.958335    -2.475921     162.25
 H      -2.552751    -4.040880    -2.403700      17.23
 C      -3.628228    -3.262798     0.020693      84.55
 H      -2.564795    -3.598092     0.346530      17.14
 O      -4.169318    -2.571249     1.065867     360.07
 H      -3.370781    -2.312856     1.530115      23.46
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 C      -4.501538    -4.545376    -0.336139      77.26
 O      -3.738814    -5.379701    -1.352070     346.39
 H      -3.352897    -5.868988    -0.588611      26.19
 H      -5.420136    -4.086645    -0.865653      26.12
 H      -4.619400    -5.190979     0.574387      26.14
55
name = lig-etoh-frame_86
 C       3.020138     1.705463    -1.905465      58.39
 H       2.988767     2.647778    -2.505383      18.11
 C       3.371572     1.063562     0.426855      57.32
 H       3.442511     1.355484     1.521817      16.97
 C       3.964089    -0.162369    -0.223127       7.49
 O       4.747277    -1.146963     0.558029     231.15
 C       5.296487    -0.617401     1.817642     108.27
 H       4.286914    -0.542346     2.526355      22.99
 H       5.851080     0.246330     1.786853      30.10
 H       5.964260    -1.347912     2.220569      26.53
 C       3.856900    -0.454859    -1.608922      21.77
 O       4.254398    -1.581581    -2.293251     172.45
 H       4.660917    -2.166901    -1.456756      22.75
 C       3.494842     0.552065    -2.506804      63.65
 H       4.024207     0.761340    -3.529785      20.81
 C       2.793114     1.936624    -0.513734      20.17
 C       2.093173     3.187858    -0.041453     121.13
 H       2.377346     3.974728    -0.674341      21.93
 O       2.365483     3.437012     1.314280     322.66
 H       3.228044     3.866630     1.260171      30.57
 C       0.551117     3.100772    -0.101811      73.22
 H       0.432871     2.992338    -1.276555      16.31
 C      -0.283752     4.438636     0.222225      98.80
 O       0.082708     5.495234    -0.580287     218.80
 H      -0.373708     5.240312    -1.567822      25.41
 H       0.023493     4.847176     1.224468      23.37
 H      -1.303646     4.005255     0.061437      19.78
 C      -1.168833    -1.265201    -0.476976      59.92
 H      -0.632293    -2.168198    -0.306728      19.00
 C      -2.986358     0.258839    -0.600253      38.17
 H      -4.100133     0.611725    -0.926271      20.39
 C      -2.191222     1.270703    -0.179155      19.64
 O      -2.685623     2.509408     0.036100     240.29
 C      -3.772238     3.343113    -0.499417     108.45
 H      -3.962675     3.263455    -1.643310      25.34
 H      -4.766506     3.267271     0.078066      24.46
 H      -3.706475     4.577215    -0.438207      23.92
 C      -0.790440     1.100853     0.092305      35.16
 O       0.227699     1.893833     0.570070     239.95
 C      -0.419600    -0.214430     0.035257      44.22
 H       0.534519    -0.427388     0.176146      18.27
 C      -2.494755    -1.048898    -0.752693      43.56
 C      -3.420777    -2.292803    -1.186529      56.01
 H      -4.342833    -1.804100    -1.601952      21.67
 O      -2.681746    -2.942126    -2.391019     244.71
 H      -2.829342    -3.889186    -2.244543      17.87
 C      -3.644810    -3.263134     0.017511      90.65
 H      -2.705258    -3.646820     0.369514      18.89
 O      -4.166126    -2.524381     1.135501     349.29
 H      -3.311044    -2.211720     1.717338      18.75
 C      -4.406977    -4.566092    -0.367356     102.57
 O      -3.773481    -5.356270    -1.358324     365.32
 H      -3.110563    -5.882819    -0.707888      24.80
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 H      -5.273761    -4.333569    -0.935064      26.68
 H      -4.690644    -5.099213     0.601023      26.48
55
name = lig-etoh-frame_87
 C       3.016917     1.806289    -1.964696      44.86
 H       2.970145     2.484771    -2.822646      20.39
 C       3.405198     1.043133     0.381819      49.43
 H       3.087830     1.180638     1.421731      15.70
 C       4.000382    -0.203281    -0.216054      25.13
 O       4.745482    -1.095866     0.547082     253.22
 C       5.253657    -0.594818     1.833343      98.97
 H       4.475361    -0.617085     2.488999      27.91
 H       5.927017     0.369540     1.685996      25.32
 H       5.821848    -1.593233     2.147040      24.35
 C       3.935089    -0.541132    -1.531906      13.58
 O       4.299862    -1.588730    -2.266126     201.95
 H       4.500149    -2.360328    -1.571813      23.87
 C       3.457342     0.562177    -2.566324      51.56
 H       3.943083     0.830719    -3.450177      23.80
 C       2.816077     1.871616    -0.511730      26.40
 C       2.069057     3.183125    -0.042469      98.35
 H       2.459805     4.114246    -0.704235      21.72
 O       2.364255     3.449279     1.303284     273.89
 H       3.361848     3.832248     1.386154      27.06
 C       0.484117     3.115153    -0.145090      91.63
 H       0.089578     2.946297    -1.101307      20.51
 C      -0.291502     4.399693     0.271768      98.72
 O       0.036297     5.545772    -0.618379     283.50
 H      -0.053442     5.418306    -1.520776      33.64
 H      -0.114681     4.674220     1.369758      24.22
 H      -1.355960     4.205420     0.063728      22.05
 C      -1.175060    -1.312932    -0.454656      47.69
 H      -0.857244    -2.405304    -0.500000      15.93
 C      -3.006839     0.239230    -0.656640      46.84
 H      -3.969322     0.457387    -0.798226      22.65
 C      -2.135922     1.278843    -0.148528      12.81
 O      -2.677367     2.614070     0.035010     220.59
 C      -3.861476     3.342887    -0.549724      99.81
 H      -3.708172     3.189406    -1.593212      25.88
 H      -4.601652     3.144479     0.350081      22.07
 H      -3.213065     4.200935    -0.303781      23.16
 C      -0.839785     1.112433     0.110725      50.39
 O       0.234591     1.887312     0.624782     214.61
 C      -0.380891    -0.176489     0.102708      35.33
 H       0.747503    -0.628693     0.168637      12.97
 C      -2.505280    -1.016464    -0.832684      25.42
 C      -3.350376    -2.341049    -1.210515      69.85
 H      -4.507656    -2.029216    -1.322623      21.38
 O      -2.711491    -2.914683    -2.281250     258.02
 H      -3.080169    -3.855071    -2.159973      16.81
 C      -3.627271    -3.273018     0.002975      79.66
 H      -2.607891    -3.712287     0.280055      20.42
 O      -4.175648    -2.488848     1.205505     331.88
 H      -3.467965    -2.062833     1.676097      25.57
 C      -4.369838    -4.542202    -0.391513      98.16
 O      -3.756885    -5.369373    -1.338652     367.48
 H      -2.944338    -5.867963    -1.207032      33.26
 H      -5.441644    -4.419414    -0.862116      25.89
 H      -4.750747    -5.049577     0.562714      24.88
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name = lig-etoh-frame_88
 C       3.026624     1.831054    -2.035246      39.76
 H       2.725076     2.611090    -2.794854      18.58
 C       3.434746     0.954680     0.303330      65.86
 H       2.983460     0.934085     1.293285      16.61
 C       4.031264    -0.213742    -0.158612      20.52
 O       4.750193    -1.055078     0.548883     239.17
 C       5.241228    -0.627639     1.821843     118.78
 H       4.415732    -0.399260     2.714333      24.95
 H       5.784414     0.275436     1.719576      28.29
 H       5.793946    -1.439153     2.094049      27.26
 C       3.953108    -0.499923    -1.578017       9.69
 O       4.366809    -1.662032    -2.221699     250.65
 H       4.485512    -2.455432    -1.824038      26.83
 C       3.441176     0.601088    -2.502914      75.97
 H       3.823479     0.496045    -3.633990      25.48
 C       2.811698     1.901050    -0.576461      51.88
 C       2.050897     3.191007    -0.079985     104.10
 H       2.426247     4.020698    -0.660549      25.01
 O       2.380743     3.480548     1.331240     307.25
 H       3.284892     3.710825     1.435456      32.15
 C       0.448219     3.127359    -0.189518      71.33
 H      -0.069187     2.812791    -1.188706      20.02
 C      -0.303768     4.364851     0.306675     106.05
 O       0.008841     5.609105    -0.611810     206.60
 H       0.244777     5.292097    -1.621671      27.23
 H      -0.205824     4.589450     1.357291      25.97
 H      -1.373222     4.335061     0.261774      24.12
 C      -1.163652    -1.312588    -0.406085      28.70
 H      -0.979553    -2.347668    -0.667474      14.42
 C      -2.999805     0.256129    -0.698079      41.26
 H      -4.201452     0.404174    -0.768838      20.75
 C      -2.208344     1.352664    -0.157271      19.36
 O      -2.634600     2.679713     0.053337     204.41
 C      -3.867970     3.331892    -0.543127     102.87
 H      -3.966573     3.015613    -1.687489      24.81
 H      -4.699598     3.097859     0.064802      25.83
 H      -3.217487     4.236142    -0.320834      22.54
 C      -0.791007     1.087625     0.175352      40.35
 O       0.202537     1.915432     0.684404     194.16
 C      -0.328017    -0.305968     0.100479       6.40
 H       0.699122    -0.316622     0.360802      16.21
 C      -2.520839    -1.070224    -0.903563      32.18
 C      -3.332697    -2.288171    -1.171203      85.57
 H      -4.445764    -2.112555    -1.391254      22.77
 O      -2.741447    -2.928799    -2.192838     233.73
 H      -3.197484    -3.876516    -2.439371      17.81
 C      -3.543730    -3.270816     0.027722      70.19
 H      -2.568346    -3.689110     0.299564      23.35
 O      -4.205399    -2.498909     1.216326     298.91
 H      -3.368108    -1.927546     1.553762      21.77
 C      -4.420097    -4.516924    -0.373591      93.69
 O      -3.731179    -5.393979    -1.358467     339.78
 H      -2.766314    -5.761498    -1.275764      28.98
 H      -5.354989    -4.268402    -0.775400      27.72
 H      -4.576035    -5.103778     0.555824      26.46
55
name = lig-etoh-frame_89
 C       3.012078     1.844467    -2.060434      11.89
 H       2.537834     2.659419    -2.551423      13.77
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 C       3.398410     0.899720     0.218691      66.15
 H       3.102142     0.816315     1.308861      17.89
 C       4.045531    -0.207461    -0.200236      10.77
 O       4.767755    -1.057904     0.581245     236.45
 C       5.196322    -0.656130     1.843665     115.06
 H       4.537553    -0.295077     2.555790      29.03
 H       5.816930     0.331972     1.738432      27.32
 H       6.038198    -1.424983     2.257473      24.99
 C       3.945132    -0.412686    -1.646476      20.50
 O       4.436579    -1.710196    -2.204523     165.60
 H       4.506802    -2.708964    -1.682408      22.82
 C       3.495669     0.578698    -2.452488      67.89
 H       3.372918     0.102206    -3.402788      22.57
 C       2.811431     1.968139    -0.678414      82.47
 C       2.042652     3.185476    -0.103687      93.87
 H       2.406014     4.084402    -0.784756      24.68
 O       2.370294     3.506602     1.359614     269.72
 H       3.391683     3.685892     1.342918      28.88
 C       0.422334     3.109186    -0.220467      70.73
 H       0.194014     2.823208    -1.216220      21.47
 C      -0.318666     4.378009     0.306053      95.18
 O      -0.007838     5.650736    -0.588158     191.39
 H       0.527501     5.056125    -1.261717      29.13
 H       0.075550     4.660454     1.393157      23.76
 H      -1.447362     4.246438     0.336325      22.59
 C      -1.184087    -1.318549    -0.397728      46.72
 H      -0.723539    -2.304068    -0.612917      15.71
 C      -3.023877     0.293274    -0.726994      37.10
 H      -4.046550     0.407142    -0.842148      20.85
 C      -2.266494     1.407455    -0.177687      -5.27
 O      -2.593191     2.700668     0.074213     220.26
 C      -3.806424     3.312922    -0.544561     118.45
 H      -4.194495     3.008128    -1.490954      26.49
 H      -4.976778     3.115688    -0.190518      23.64
 H      -3.888190     4.521161    -0.600835      24.71
 C      -0.760708     0.997951     0.240683      -2.11
 O       0.139895     1.966657     0.740920     163.32
 C      -0.303246    -0.391675     0.084635      29.80
 H       0.758682    -0.296881     0.541704      15.18
 C      -2.491987    -1.072105    -0.904745      33.56
 C      -3.392170    -2.222117    -1.079867      76.74
 H      -4.380586    -1.886089    -1.610834      21.25
 O      -2.737968    -2.995483    -2.187980     262.50
 H      -3.207392    -3.694563    -2.486797      24.94
 C      -3.474023    -3.253759     0.084779      78.09
 H      -2.494958    -3.632546     0.467541      20.76
 O      -4.203512    -2.540513     1.177586     339.21
 H      -3.444304    -1.957105     1.460423      25.19
 C      -4.427021    -4.499505    -0.325173      71.36
 O      -3.716513    -5.413013    -1.408711     325.63
 H      -2.888082    -5.487299    -0.851786      25.99
 H      -5.381732    -4.079109    -0.830073      25.89
 H      -4.404782    -5.203434     0.603861      25.43
55
name = lig-etoh-frame_90
 C       2.980199     1.849160    -2.038249      72.04
 H       2.449525     2.611009    -2.710560      22.15
 C       3.297343     0.918789     0.163863      50.22
 H       3.300076     1.020015     1.223849      20.77
 C       4.066450    -0.199848    -0.307444       3.56
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 O       4.775835    -1.099756     0.600538     234.90
 C       5.236986    -0.641871     1.884009     113.52
 H       4.300596    -0.389711     2.621771      24.09
 H       5.817927     0.245873     1.698645      27.98
 H       5.867673    -1.311441     2.322377      26.65
 C       3.992044    -0.426679    -1.646078      27.84
 O       4.497654    -1.738172    -2.202956     199.31
 H       4.412719    -2.285761    -1.378558      25.66
 C       3.530996     0.532264    -2.483341      66.56
 H       2.975433     0.031499    -3.365172      19.16
 C       2.832734     2.001146    -0.716028      23.46
 C       2.038506     3.201635    -0.108261      96.98
 H       2.274718     4.082108    -0.747471      25.18
 O       2.363033     3.525382     1.350022     276.30
 H       3.374694     3.717740     1.271958      26.49
 C       0.440992     3.080472    -0.202101      60.83
 H       0.343658     2.824927    -1.324924      19.48
 C      -0.311691     4.438280     0.314339     115.43
 O      -0.010475     5.634434    -0.540025     259.66
 H       0.614911     5.292214    -1.096453      34.64
 H       0.251979     4.621425     1.154247      26.87
 H      -1.314945     4.185505     0.355131      25.73
 C      -1.187958    -1.372684    -0.431216      57.19
 H      -0.617261    -2.302275    -0.454751      14.67
 C      -3.016311     0.334382    -0.739638      41.21
 H      -4.143709     0.495286    -1.024980      18.46
 C      -2.231494     1.367920    -0.194309       4.80
 O      -2.599077     2.738531     0.081052     224.35
 C      -3.815815     3.325407    -0.549826     122.11
 H      -3.933665     2.831384    -1.629088      25.76
 H      -4.659322     3.035549     0.034246      27.16
 H      -4.237319     4.267857    -0.762489      26.62
 C      -0.803155     0.917277     0.274047       8.48
 O       0.052826     2.013800     0.781352     185.48
 C      -0.285535    -0.340502     0.103076      56.74
 H       0.702773    -0.779799     0.533742      16.68
 C      -2.448865    -0.996307    -0.836320      26.90
 C      -3.442102    -2.200725    -1.055841      64.30
 H      -4.363453    -1.731559    -1.439401      24.28
 O      -2.702595    -3.041425    -2.206581     164.46
 H      -3.426829    -3.801115    -2.444086      18.26
 C      -3.473796    -3.234299     0.138004      89.25
 H      -2.449671    -3.500079     0.521308      22.22
 O      -4.185901    -2.599250     1.122380     372.62
 H      -3.591981    -1.980654     1.584152      28.40
 C      -4.381408    -4.487055    -0.292520      93.65
 O      -3.712321    -5.400930    -1.417528     348.86
 H      -3.073311    -5.501327    -0.703303      26.96
 H      -5.310964    -4.116565    -0.653943      28.45
 H      -4.567070    -5.113942     0.536818      28.07
55
name = lig-etoh-frame_91
 C       2.954019     1.802327    -2.077058      61.64
 H       2.582702     2.321694    -2.921702      25.64
 C       3.226261     0.952016     0.119573      69.15
 H       3.419726     1.371642     1.177217      18.84
 C       4.081625    -0.160155    -0.319539       8.83
 O       4.765727    -1.149806     0.584937     223.09
 C       5.239310    -0.581678     1.928050      92.58
 H       4.342435    -0.602688     2.509488      24.94
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 H       5.838226     0.348653     1.763460      25.50
 H       5.806905    -1.526184     2.430782      23.52
 C       4.093909    -0.528554    -1.683354       5.44
 O       4.532785    -1.719819    -2.174169     230.72
 H       4.478431    -2.060014    -1.250101      23.71
 C       3.484968     0.524793    -2.572943      45.48
 H       2.921797     0.265523    -3.469806      18.53
 C       2.842463     2.018564    -0.654511      29.54
 C       2.019462     3.219300    -0.076151     113.40
 H       2.239187     4.175731    -0.714962      22.37
 O       2.368642     3.537240     1.298331     325.88
 H       3.266365     3.804089     1.355273      31.30
 C       0.483872     3.055813    -0.171009      62.07
 H       0.201130     2.798504    -1.190461      21.60
 C      -0.237930     4.479050     0.285551      96.53
 O      -0.024162     5.607342    -0.478562     210.79
 H       0.748554     5.606839    -1.239382      27.02
 H       0.341945     4.608301     1.348973      23.03
 H      -1.353125     4.256625     0.455899      22.58
 C      -1.126859    -1.371062    -0.446212      26.91
 H      -0.911938    -2.460300    -0.432959      16.82
 C      -3.004595     0.374306    -0.742731      47.44
 H      -3.987131     0.570015    -1.201799      19.93
 C      -2.151416     1.311839    -0.192568       2.16
 O      -2.599103     2.777127     0.078447     179.89
 C      -3.873972     3.246532    -0.597656      86.10
 H      -3.672913     2.730284    -1.484714      26.26
 H      -4.397341     2.699739     0.351899      19.99
 H      -3.882528     4.455081    -0.722968      23.99
 C      -0.869695     0.949255     0.289531       1.81
 O      -0.051771     2.041465     0.802269     205.17
 C      -0.303050    -0.332159     0.120661      59.73
 H       0.557040    -0.778000     0.431718      16.23
 C      -2.459353    -0.958577    -0.756502      32.20
 C      -3.395071    -2.201557    -1.092302      37.01
 H      -4.539055    -1.787394    -1.153432      24.03
 O      -2.697317    -3.061974    -2.227125     167.40
 H      -3.349416    -3.860787    -2.266476      17.57
 C      -3.490078    -3.222758     0.128323     103.73
 H      -2.463843    -3.444380     0.388869      24.53
 O      -4.201005    -2.645820     1.109936     331.38
 H      -3.681014    -2.029940     1.780189      26.45
 C      -4.310891    -4.475478    -0.287125      89.25
 O      -3.729730    -5.355545    -1.366978     294.07
 H      -2.928760    -5.975695    -0.920527      23.91
 H      -5.361427    -4.115191    -0.605022      26.86
 H      -4.768917    -5.112370     0.631809      25.56
55
name = lig-etoh-frame_92
 C       2.945863     1.695710    -2.122921      29.98
 H       2.598583     2.300458    -3.026897      21.44
 C       3.248366     0.979000     0.141062      70.17
 H       3.364243     1.380951     1.105213      21.73
 C       4.087986    -0.128922    -0.289589      16.69
 O       4.745056    -1.162720     0.558771     210.36
 C       5.233397    -0.585341     1.941494      99.15
 H       4.278121    -0.476476     2.582493      24.09
 H       5.779129     0.404316     1.967467      26.11
 H       5.776796    -1.402140     2.290114      25.68
 C       4.141372    -0.520438    -1.765391      -2.41
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 O       4.561025    -1.708120    -2.126321     157.55
 H       4.896494    -2.382741    -1.246049      18.21
 C       3.419738     0.508558    -2.621523      54.00
 H       3.203800     0.380521    -3.740285      23.22
 C       2.816168     2.049195    -0.653715      41.65
 C       2.021607     3.236781    -0.046778     107.90
 H       2.222659     4.130528    -0.707158      20.82
 O       2.366713     3.541658     1.250953     300.22
 H       3.332529     3.957584     1.371184      27.55
 C       0.486061     3.057218    -0.122371      64.30
 H       0.063548     2.747470    -1.100923      21.14
 C      -0.121236     4.447004     0.314760     115.67
 O      -0.027463     5.624331    -0.446424     257.44
 H       0.607071     5.654249    -1.237960      29.92
 H       0.143877     4.625727     1.287279      26.87
 H      -1.160486     4.418451     0.467419      26.18
 C      -1.100628    -1.319611    -0.441205      42.02
 H      -1.137272    -2.399256    -0.478755      16.50
 C      -2.966351     0.366931    -0.749867      49.20
 H      -3.894553     0.637477    -1.258792      22.25
 C      -2.111506     1.343162    -0.172426      -4.35
 O      -2.547011     2.775998     0.068974     169.54
 C      -3.899021     3.140643    -0.583397     109.79
 H      -3.865371     2.630738    -1.664426      25.67
 H      -4.637839     2.743919     0.019977      27.79
 H      -3.495147     4.088467    -0.515683      25.85
 C      -0.880413     1.041805     0.297111      13.08
 O      -0.151240     2.056133     0.819841     224.12
 C      -0.365912    -0.358942     0.120610      25.50
 H       0.869272    -0.378999     0.519056      13.56
 C      -2.502960    -0.986520    -0.711511      35.02
 C      -3.321026    -2.210061    -1.130852      74.38
 H      -4.400311    -2.005060    -1.230681      23.83
 O      -2.722786    -3.042338    -2.232936     222.33
 H      -3.086866    -3.952432    -2.168068      18.26
 C      -3.472642    -3.224115     0.051981      98.96
 H      -2.409330    -3.559538     0.334797      22.11
 O      -4.260533    -2.666646     1.159964     328.27
 H      -3.610119    -2.201748     1.690352      28.25
 C      -4.282573    -4.495568    -0.272864     101.72
 O      -3.738346    -5.319516    -1.283917     362.11
 H      -3.204297    -6.053428    -1.223055      32.75
 H      -5.173716    -4.120847    -0.782811      27.78
 H      -4.510423    -5.002970     0.580813      28.01
55
name = lig-etoh-frame_93
 C       2.904784     1.640580    -2.136666      69.17
 H       2.547960     2.412666    -2.787285      19.29
 C       3.340464     1.007494     0.186291      20.98
 H       3.252206     1.145929     1.339979      17.23
 C       4.085465    -0.128713    -0.307568      -1.50
 O       4.720488    -1.115869     0.544893     212.17
 C       5.177726    -0.606176     1.923543      98.78
 H       4.338128    -0.311641     2.624403      25.29
 H       5.723228     0.337176     1.947348      27.88
 H       5.939290    -1.416284     2.291967      24.77
 C       4.112027    -0.403622    -1.760055      13.27
 O       4.615264    -1.751787    -2.087829     236.26
 H       5.126724    -2.235242    -1.585796      26.40
 C       3.394357     0.418821    -2.667626      75.71
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 H       3.770630     0.386173    -3.731881      27.40
 C       2.784878     2.030142    -0.746177      19.11
 C       2.037138     3.222284    -0.074486     103.57
 H       2.205479     4.118147    -0.796263      21.48
 O       2.384362     3.555663     1.253372     299.19
 H       3.275773     3.968141     1.177386      28.71
 C       0.447185     3.079150    -0.072666      69.91
 H       0.128988     2.787736    -1.119781      19.46
 C      -0.042049     4.390099     0.368551      96.71
 O      -0.013749     5.679549    -0.439890     234.75
 H       0.454427     5.455763    -1.218201      32.80
 H       0.282953     4.714168     1.474328      23.48
 H      -1.167245     4.279568     0.396655      22.92
 C      -1.173445    -1.281659    -0.430223      50.63
 H      -0.807289    -2.351685    -0.506058      17.52
 C      -2.912849     0.326905    -0.749262      51.55
 H      -3.931745     0.675656    -1.224493      22.84
 C      -2.150218     1.431771    -0.153715       1.11
 O      -2.494980     2.704714     0.040156     188.21
 C      -3.855019     3.001313    -0.583400     109.48
 H      -4.148757     2.819775    -1.591796      27.18
 H      -5.067939     2.888726    -0.196430      23.58
 H      -3.641565     4.173108    -0.495974      24.46
 C      -0.846432     1.071231     0.280180      14.55
 O      -0.202460     2.090805     0.861836     223.24
 C      -0.338835    -0.284953     0.165016      28.44
 H       0.582957    -0.176467     0.395272      18.88
 C      -2.530037    -1.015979    -0.714911      35.21
 C      -3.264581    -2.252950    -1.150686      76.24
 H      -4.342651    -2.023581    -1.665105      19.22
 O      -2.751361    -2.989592    -2.247653     216.92
 H      -2.720158    -4.056086    -1.979826      15.09
 C      -3.433052    -3.243476    -0.002142     104.86
 H      -2.516641    -3.613257     0.403380      21.73
 O      -4.303742    -2.689076     1.202863     287.78
 H      -3.507590    -2.248908     1.616122      24.12
 C      -4.264026    -4.496950    -0.275147      81.60
 O      -3.752527    -5.288590    -1.258946     318.74
 H      -3.297245    -6.163843    -0.967700      28.70
 H      -5.190090    -4.142959    -0.818706      24.77
 H      -4.289683    -5.042450     0.813678      24.36
55
name = lig-etoh-frame_94
 C       2.835557     1.634449    -2.129396      59.51
 H       2.469087     2.489760    -2.744392      19.63
 C       3.448813     1.042445     0.220123      41.46
 H       3.153762     0.913300     1.230396      18.21
 C       4.064608    -0.115965    -0.324485       0.47
 O       4.696364    -1.034803     0.544914     225.97
 C       5.125896    -0.629817     1.884293     102.34
 H       4.334902    -0.458606     2.623356      27.14
 H       5.751175     0.311337     1.648331      25.74
 H       5.849252    -1.369929     2.304267      25.78
 C       4.086696    -0.359832    -1.680986       3.62
 O       4.637964    -1.747489    -2.103016     131.31
 H       5.514258    -2.044171    -1.464990      22.57
 C       3.435121     0.338264    -2.702655      57.95
 H       3.985158     0.302515    -3.618345      25.54
 C       2.783281     1.925594    -0.797856      28.51
 C       2.033436     3.177935    -0.148033     102.47
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 H       2.164267     4.091356    -0.817929      22.18
 O       2.422714     3.569818     1.259331     283.82
 H       3.327703     3.923315     1.152946      30.06
 C       0.447141     3.086258    -0.053240      81.69
 H       0.185279     2.905693    -1.079832      19.25
 C      -0.062651     4.413493     0.466476      96.93
 O       0.026214     5.719272    -0.432382     176.40
 H       0.256890     5.202565    -1.399489      26.14
 H       0.478515     4.606752     1.311731      25.63
 H      -1.095748     4.098064     0.493167      22.25
 C      -1.207062    -1.255048    -0.380173      57.62
 H      -0.558228    -2.076494    -0.543485      18.66
 C      -2.901829     0.340021    -0.738857      72.11
 H      -3.861381     0.513096    -1.060868      27.07
 C      -2.175072     1.391211    -0.156159      12.69
 O      -2.519592     2.635847    -0.012978     231.73
 C      -3.841886     2.973450    -0.566657     131.46
 H      -3.982550     2.842229    -1.725993      26.35
 H      -4.700850     2.830095    -0.037855      27.86
 H      -4.083947     4.014994    -0.624077      27.01
 C      -0.854446     1.061463     0.241853      43.94
 O      -0.188606     2.156085     0.923430     199.71
 C      -0.364844    -0.159447     0.184703      16.87
 H       0.936409    -0.358517     0.395244      14.90
 C      -2.510136    -1.040473    -0.749491      30.57
 C      -3.292429    -2.290052    -1.185450      89.74
 H      -4.197053    -1.890095    -1.647590      20.96
 O      -2.732540    -2.967996    -2.285044     281.00
 H      -2.493041    -3.765808    -1.934241      25.26
 C      -3.447742    -3.266212     0.003050     101.41
 H      -2.445537    -3.554836     0.510262      19.03
 O      -4.296419    -2.713626     1.211940     274.64
 H      -3.551265    -2.126353     1.681573      22.95
 C      -4.279097    -4.471681    -0.242151     101.15
 O      -3.727494    -5.324048    -1.289349     349.34
 H      -3.396773    -5.954085    -0.529132      25.35
 H      -5.358125    -4.208061    -0.405230      26.18
 H      -4.311821    -4.951042     0.643722      27.65
55
name = lig-etoh-frame_95
 C       2.782857     1.606894    -2.172715      64.06
 H       2.398095     2.338905    -2.892381      19.22
 C       3.520715     1.064389     0.184724      75.33
 H       3.123032     1.008525     1.228545      15.15
 C       4.049210    -0.081678    -0.269245      17.01
 O       4.669232    -0.977553     0.538558     251.13
 C       5.100579    -0.615203     1.813278     110.57
 H       4.231352    -0.607038     2.615094      25.54
 H       5.645778     0.266359     1.643492      27.25
 H       5.721152    -1.464065     2.216862      25.08
 C       4.083993    -0.438740    -1.649404      11.65
 O       4.664247    -1.708148    -2.103293     174.57
 H       5.532532    -1.548099    -1.511525      22.97
 C       3.490551     0.350609    -2.666747      45.68
 H       3.895249     0.166600    -3.753888      23.95
 C       2.790804     1.815713    -0.740177      46.62
 C       2.019267     3.117570    -0.198427     103.52
 H       2.191466     4.020410    -0.839739      22.67
 O       2.470942     3.570663     1.232673     257.21
 H       3.507899     3.840182     1.272368      29.47
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 C       0.492142     3.099980    -0.049236      76.74
 H       0.009835     2.925572    -1.099748      18.65
 C      -0.117325     4.479895     0.523439      80.17
 O       0.078823     5.693487    -0.435933     220.10
 H      -0.031807     5.377620    -1.313499      32.01
 H       0.618325     4.638966     1.424753      23.12
 H      -1.175628     4.277211     0.836101      22.98
 C      -1.144688    -1.187671    -0.297267      62.73
 H      -0.542865    -2.110472    -0.608501      17.42
 C      -2.934095     0.326278    -0.727433      60.29
 H      -4.104456     0.435353    -0.960191      21.81
 C      -2.170643     1.255737    -0.180734      24.02
 O      -2.601813     2.633481    -0.072986     193.50
 C      -3.835682     2.994255    -0.596904      90.38
 H      -3.694429     2.553127    -1.581251      24.90
 H      -4.535829     2.280067     0.359700      20.20
 H      -4.069578     4.114493    -0.595949      23.09
 C      -0.867434     1.138096     0.251339      39.46
 O      -0.145812     2.206451     0.960998     213.08
 C      -0.335305    -0.137325     0.171919      -3.86
 H       0.516685    -0.444688     0.355329      20.90
 C      -2.456211    -1.052938    -0.789106      61.00
 C      -3.340810    -2.279387    -1.206246      67.97
 H      -4.419959    -1.746032    -1.406458      23.48
 O      -2.684871    -2.950301    -2.346843     217.26
 H      -2.252267    -3.816859    -1.961639      22.77
 C      -3.491544    -3.258559     0.071513     114.96
 H      -2.489099    -3.428790     0.364205      28.00
 O      -4.246388    -2.724207     1.196226     323.76
 H      -3.768928    -2.087486     1.667242      31.46
 C      -4.335603    -4.443017    -0.228221      88.89
 O      -3.698739    -5.382900    -1.289796     327.52
 H      -3.230105    -5.922983    -0.678039      30.73
 H      -5.413550    -4.221334    -0.167949      27.35
 H      -4.346073    -5.123088     0.794899      26.47
55
name = lig-etoh-frame_96
 C       2.776524     1.521172    -2.207076      55.49
 H       2.298265     2.124443    -2.983461      24.83
 C       3.522970     1.096907     0.169546      48.86
 H       3.340083     1.398048     1.228698      14.80
 C       4.067210    -0.095082    -0.247155      26.56
 O       4.645808    -0.972602     0.519032     243.33
 C       5.071507    -0.607538     1.781795     113.38
 H       4.242786    -0.538836     2.440750      28.27
 H       5.630746     0.426411     1.962000      26.48
 H       5.699295    -1.550719     2.038914      24.52
 C       4.059429    -0.539903    -1.674684      25.88
 O       4.704143    -1.622278    -2.076826     260.59
 H       5.504669    -1.558395    -1.669309      28.22
 C       3.543318     0.422133    -2.599721      59.50
 H       3.494238     0.112341    -3.611807      20.25
 C       2.756677     1.787528    -0.715077      42.60
 C       2.030286     3.061735    -0.190530     100.22
 H       2.319730     3.902408    -0.967891      19.66
 O       2.529928     3.555836     1.182167     302.73
 H       3.455771     3.681186     1.211400      32.74
 C       0.481951     3.151427    -0.054668      70.84
 H      -0.031698     2.908802    -0.923306      22.55
 C      -0.126664     4.557480     0.552292      95.63
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 O       0.117684     5.642887    -0.403307     236.18
 H      -0.202065     5.453490    -1.336433      29.33
 H       0.504404     4.828455     1.386069      25.45
 H      -1.121947     4.620194     1.052468      24.83
 C      -1.068863    -1.164552    -0.267400      53.32
 H      -0.721359    -2.138604    -0.455658      18.28
 C      -3.044012     0.200059    -0.742064      57.05
 H      -4.008860     0.468027    -0.863728      20.60
 C      -2.178782     1.260878    -0.192856      10.56
 O      -2.624397     2.640855    -0.109151     199.28
 C      -3.884308     2.950910    -0.583261     127.90
 H      -3.938557     2.356187    -1.569134      24.61
 H      -4.385301     2.306910    -0.111748      29.16
 H      -3.898285     4.021621    -0.477708      25.43
 C      -0.828161     1.221768     0.316552       9.70
 O      -0.101958     2.217599     0.961538     221.79
 C      -0.341301    -0.126827     0.147289      36.79
 H       0.859224    -0.485148     0.578089      14.84
 C      -2.407755    -1.039061    -0.813884      27.70
 C      -3.380011    -2.222885    -1.192482      66.47
 H      -4.394300    -1.945815    -1.378933      25.69
 O      -2.641309    -2.932312    -2.400463     180.90
 H      -2.247423    -3.840786    -2.054181      20.67
 C      -3.540056    -3.214032     0.120271      82.90
 H      -2.421406    -3.497858     0.281015      23.16
 O      -4.206769    -2.728993     1.171123     316.05
 H      -3.718413    -1.942946     1.631807      27.15
 C      -4.374074    -4.509773    -0.176567      86.65
 O      -3.696002    -5.417222    -1.267859     313.65
 H      -2.927290    -6.040431    -0.898134      27.38
 H      -5.465086    -4.206122    -0.428027      26.11
 H      -4.276485    -5.091582     0.652167      28.44
55
name = lig-etoh-frame_97
 C       2.775718     1.449238    -2.158837      75.92
 H       2.156522     1.943531    -2.943124      23.50
 C       3.496798     1.127363     0.185822      49.75
 H       3.721022     1.643461     1.135701      17.40
 C       4.074351    -0.119773    -0.324640      10.84
 O       4.656160    -1.013684     0.505698     214.53
 C       5.074389    -0.601551     1.807924     117.19
 H       4.067132    -0.502033     2.463469      23.97
 H       5.581743     0.281940     2.031910      28.42
 H       5.708878    -1.402340     2.079201      26.24
 C       4.003977    -0.528435    -1.655059      40.19
 O       4.751048    -1.569023    -2.069756     171.53
 H       5.793908    -1.839048    -1.693096      24.43
 C       3.575544     0.452852    -2.543344      71.41
 H       3.177237     0.084844    -3.573320      20.14
 C       2.680799     1.826237    -0.777260      10.18
 C       2.061563     3.054846    -0.161425     113.78
 H       2.340029     3.753179    -0.944048      20.42
 O       2.565244     3.519633     1.111699     290.43
 H       3.596393     3.620378     0.996966      28.73
 C       0.428319     3.233692    -0.011382      48.94
 H      -0.054711     2.937368    -1.056084      20.29
 C      -0.085889     4.638699     0.552625     105.81
 O       0.150561     5.602173    -0.363572     217.03
 H      -0.342810     5.409238    -1.308037      26.95
 H       0.582398     4.952330     1.377961      25.43
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 H      -1.120492     4.664713     0.930286      25.53
 C      -1.063293    -1.199962    -0.312223      49.53
 H      -0.696071    -2.280864    -0.165596      16.53
 C      -3.078253     0.126965    -0.719597      38.80
 H      -4.194716     0.412855    -0.942335      18.13
 C      -2.197513     1.351844    -0.192949       0.48
 O      -2.584668     2.628172    -0.128482     175.42
 C      -3.925049     2.869696    -0.624258     105.89
 H      -4.289080     2.709796    -1.692928      24.93
 H      -5.054058     2.302656    -0.024299      21.84
 H      -4.045643     3.974372    -0.467479      26.01
 C      -0.806287     1.218165     0.368069      -4.14
 O      -0.059288     2.206578     0.947599     215.24
 C      -0.250388    -0.086876     0.184636      43.60
 H       0.625131    -0.125726     0.613645      19.36
 C      -2.406730    -1.041785    -0.822535      36.97
 C      -3.338212    -2.195103    -1.153322      62.06
 H      -4.437109    -2.050292    -1.691273      21.31
 O      -2.615748    -2.907159    -2.429326     205.89
 H      -2.514756    -3.756630    -2.120378      23.60
 C      -3.530275    -3.218624     0.071127      85.17
 H      -2.582742    -3.615407     0.355231      23.72
 O      -4.194926    -2.691030     1.190373     316.62
 H      -3.552482    -1.944102     1.477594      25.62
 C      -4.360079    -4.599733    -0.177382      83.91
 O      -3.710860    -5.435387    -1.239094     331.76
 H      -2.864467    -5.880655    -0.898377      26.92
 H      -5.263384    -4.399557    -0.735923      25.21
 H      -4.358364    -5.211023     0.864756      24.98
55
name = lig-etoh-frame_98
 C       2.715932     1.456196    -2.069862      68.17
 H       2.054162     1.850453    -2.806823      23.50
 C       3.466715     1.125062     0.147721      69.49
 H       4.071578     1.615447     0.968138      21.52
 C       4.053177    -0.092748    -0.343097      11.19
 O       4.701001    -1.067754     0.498680     202.29
 C       5.029013    -0.612237     1.868544     100.93
 H       4.194514    -0.594650     2.455003      27.18
 H       5.662343     0.400774     1.814460      24.63
 H       5.789134    -1.411574     2.389682      24.47
 C       4.009333    -0.478294    -1.618600      32.72
 O       4.817738    -1.569072    -2.098257     217.99
 H       5.581421    -1.850219    -1.551233      27.23
 C       3.555334     0.403720    -2.567271      52.82
 H       3.340685     0.105372    -3.539338      20.69
 C       2.631447     1.852652    -0.789781      22.57
 C       2.040571     3.107543    -0.153269     113.28
 H       2.281338     3.964237    -0.971241      20.05
 O       2.617371     3.470472     1.039797     307.37
 H       3.591970     3.737207     0.857792      28.86
 C       0.379513     3.290128     0.025197      76.12
 H       0.053362     3.189181    -0.950574      22.67
 C      -0.023704     4.664429     0.576079     113.95
 O       0.177370     5.617630    -0.380407     278.47
 H      -0.259248     5.354586    -1.122251      34.33
 H       0.698191     4.862202     1.454621      24.96
 H      -1.119850     4.462208     0.757977      24.75
 C      -1.049300    -1.231769    -0.357682      35.19
 H      -0.770612    -2.178341     0.006042      19.73
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 C      -3.057073     0.217026    -0.657823      42.04
 H      -4.063097     0.141221    -1.058424      20.46
 C      -2.189134     1.364411    -0.182746       2.74
 O      -2.596988     2.633856    -0.165832     171.43
 C      -4.054505     2.811705    -0.648362     127.26
 H      -4.190344     2.994629    -1.735045      25.84
 H      -4.715340     2.670516     0.000410      29.34
 H      -4.242419     3.880409    -0.422960      27.29
 C      -0.848194     1.150908     0.361428       7.09
 O      -0.022702     2.197857     0.933982     182.70
 C      -0.234844    -0.058946     0.215396      33.07
 H       0.941368    -0.056873     0.782854      14.73
 C      -2.417441    -1.076167    -0.802415      20.56
 C      -3.281421    -2.235658    -1.167945      87.42
 H      -4.109223    -1.905865    -1.658074      24.65
 O      -2.603394    -2.867043    -2.426358     182.87
 H      -2.874230    -3.915441    -2.211058      17.57
 C      -3.526690    -3.291441    -0.012165      79.39
 H      -2.528936    -3.668492     0.442231      20.97
 O      -4.183854    -2.621829     1.212554     293.82
 H      -3.495703    -2.033361     1.504229      25.88
 C      -4.298912    -4.687016    -0.206991     100.40
 O      -3.713854    -5.450749    -1.204425     357.16
 H      -2.938577    -5.761745    -0.731488      30.33
 H      -5.293347    -4.563096    -0.788916      24.43
 H      -4.635447    -5.066529     0.741197      27.03
55
name = lig-etoh-frame_99
 C       2.633301     1.458170    -2.054587      61.40
 H       1.921111     1.956416    -2.778703      21.09
 C       3.471195     1.103088     0.085706      65.75
 H       4.011885     1.495733     0.892258      17.56
 C       4.034565    -0.065108    -0.246394      31.01
 O       4.755746    -1.104889     0.507242     229.63
 C       5.043946    -0.628436     1.913424     118.77
 H       4.051834    -0.551715     2.622896      24.07
 H       5.470724     0.283717     1.682782      27.88
 H       5.634126    -1.277352     2.406105      27.83
 C       4.099704    -0.479235    -1.656471      16.98
 O       4.853505    -1.567934    -2.136253     198.38
 H       5.368105    -1.781566    -1.278328      22.84
 C       3.462420     0.363432    -2.595590      72.70
 H       3.672391     0.100612    -3.731048      19.92
 C       2.616042     1.876383    -0.700539      42.33
 C       1.967450     3.220855    -0.217808     117.78
 H       2.136518     4.053398    -0.840479      23.40
 O       2.689122     3.432426     0.999845     321.22
 H       3.515205     3.869561     0.885541      33.42
 C       0.412091     3.299860     0.061640      77.44
 H      -0.066091     3.320358    -1.030499      18.71
 C       0.029560     4.617840     0.632615     111.38
 O       0.213293     5.683459    -0.411055     195.80
 H      -0.186381     5.304362    -1.280772      29.11
 H       0.588888     4.799730     1.494550      26.68
 H      -1.019888     4.444786     0.857708      24.64
 C      -1.022768    -1.204036    -0.360638      35.63
 H      -0.818881    -2.243581    -0.029956      21.34
 C      -2.959226     0.306180    -0.601580      49.15
 H      -3.962673     0.273502    -1.069858      21.14
 C      -2.196877     1.303654    -0.175159      10.01
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 O      -2.669757     2.670728    -0.220615     161.34
 C      -4.120223     2.863382    -0.674099      86.29
 H      -4.063957     2.752730    -1.789091      24.18
 H      -4.842571     2.306396     0.370227      20.26
 H      -4.168727     3.954178    -0.387634      24.81
 C      -0.890735     1.114467     0.327900       3.66
 O      -0.017581     2.185954     0.912552     178.60
 C      -0.239287    -0.109520     0.243951      39.78
 H       0.728584    -0.244360     0.572158      17.42
 C      -2.387436    -1.066718    -0.728893      31.81
 C      -3.196445    -2.316602    -1.215323      60.01
 H      -4.228318    -1.617304    -1.503958      21.44
 O      -2.607035    -2.868873    -2.385011     247.47
 H      -3.111894    -3.685003    -2.617461      22.30
 C      -3.522820    -3.381084    -0.032503      82.29
 H      -2.523706    -3.580521     0.299229      21.38
 O      -4.174014    -2.570300     1.185335     233.72
 H      -3.344409    -2.063715     1.678869      19.82
 C      -4.323819    -4.677157    -0.278997     102.47
 O      -3.672757    -5.496830    -1.175508     366.76
 H      -2.843743    -5.974182    -0.647281      25.24
 H      -5.344222    -4.444839    -0.560214      25.75
 H      -4.658049    -5.126328     0.751101      24.99
55
name = lig-etoh-frame_100
 C       2.539712     1.444540    -2.090397      31.01
 H       1.951329     2.066116    -2.734848      19.00
 C       3.495197     1.109562     0.094896      51.64
 H       3.660376     1.531709     1.178096      14.89
 C       4.057171    -0.151848    -0.228294      13.75
 O       4.797146    -1.109827     0.546556     251.37
 C       5.009233    -0.642021     1.933417      98.25
 H       4.152033    -0.465275     2.448506      27.91
 H       5.459941     0.440397     1.849084      25.34
 H       5.803666    -1.434450     2.459258      24.39
 C       4.176174    -0.459811    -1.714484      -8.71
 O       4.893969    -1.553863    -2.149851     165.83
 H       5.050531    -1.927858    -1.077581      17.85
 C       3.349414     0.333646    -2.614184      67.19
 H       3.800811     0.302908    -3.577339      26.81
 C       2.594514     1.898289    -0.675413      36.90
 C       1.919566     3.296644    -0.263201     100.19
 H       2.106737     4.267775    -0.989188      18.86
 O       2.741911     3.411564     0.996831     262.93
 H       3.572735     4.083397     0.889161      28.00
 C       0.471714     3.264682     0.038326      90.72
 H      -0.132961     3.213433    -0.805612      19.15
 C       0.050375     4.579091     0.665331      83.36
 O       0.235259     5.742197    -0.415699     126.52
 H       0.133175     5.317012    -1.416514      25.72
 H       0.645058     4.943038     1.632068      22.84
 H      -1.009705     4.618382     1.059560      22.92
 C      -1.009918    -1.181150    -0.314920      47.85
 H      -0.750508    -2.267960    -0.335023      20.04
 C      -2.885909     0.250655    -0.604460      55.39
 H      -3.890060     0.721494    -0.963527      22.31
 C      -2.203921     1.346546    -0.149788       8.97
 O      -2.748215     2.692148    -0.274971     224.96
 C      -4.148121     2.914332    -0.613356     125.21
 H      -4.289622     2.373301    -1.600972      25.89
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 H      -4.621225     2.186287    -0.216521      29.45
 H      -4.210144     4.027132    -0.513739      24.53
 C      -0.860235     1.122663     0.302536      29.34
 O      -0.044616     2.160062     0.882227     194.04
 C      -0.314861    -0.195252     0.232697      36.28
 H       0.864443    -0.443589     0.535188      15.57
 C      -2.329235    -1.026482    -0.641179      50.60
 C      -3.186583    -2.326708    -1.235684      71.09
 H      -4.119888    -1.912186    -1.322895      24.16
 O      -2.613586    -2.885417    -2.359695     300.49
 H      -3.215129    -3.442938    -2.856695      25.79
 C      -3.509366    -3.401729    -0.008187      78.10
 H      -2.444647    -3.712788     0.248348      17.54
 O      -4.141653    -2.547257     1.113255     309.95
 H      -3.406559    -2.217564     1.607601      24.07
 C      -4.394782    -4.622340    -0.295200      86.11
 O      -3.604705    -5.573070    -1.166072     385.67
 H      -3.021561    -6.146059    -0.686066      29.15
 H      -5.441289    -4.241480    -0.617883      25.82
 H      -4.321115    -5.211024     0.641257      25.04
55
name = lig-etoh-frame_103
 C       2.430827     1.407322    -2.141068      63.54
 H       1.878658     1.941158    -2.935831      27.19
 C       3.374699     0.976450     0.128502      53.83
 H       3.279632     1.037345     1.193564      19.99
 C       4.104390    -0.085144    -0.261777      17.24
 O       4.856855    -1.008364     0.561899     206.27
 C       5.004489    -0.656924     2.001062     119.21
 H       3.980761    -0.711468     2.626345      24.85
 H       5.523560     0.311906     2.063225      27.13
 H       5.493261    -1.450017     2.379679      28.08
 C       4.105373    -0.451775    -1.690788      25.26
 O       4.994000    -1.459316    -2.158234     235.02
 H       4.718840    -2.375201    -1.746676      27.89
 C       3.216762     0.338917    -2.555587      67.89
 H       2.965741    -0.079026    -3.555091      18.97
 C       2.675109     1.826662    -0.781211      19.84
 C       2.189358     3.105717    -0.212284     109.85
 H       2.407208     3.811866    -0.874229      21.35
 O       2.720318     3.543523     1.012335     281.55
 H       3.768216     3.777987     0.921695      26.31
 C       0.424015     3.253527    -0.017708      63.41
 H       0.106401     3.160282    -1.088271      19.28
 C       0.163631     4.693581     0.574969     119.59
 O       0.226998     5.746700    -0.311788     256.00
 H       0.880121     5.467877    -0.970028      32.28
 H       0.778537     4.710580     1.432729      26.02
 H      -0.808296     4.624098     1.040202      25.94
 C      -1.036162    -1.368089    -0.258814      54.36
 H      -0.474380    -2.157948    -0.688797      16.57
 C      -2.912032     0.278713    -0.619306      43.54
 H      -3.840182     0.211147    -0.913066      23.08
 C      -2.196232     1.409544    -0.199490       3.83
 O      -2.711734     2.752688    -0.333105     180.02
 C      -4.241477     2.814657    -0.595533     105.81
 H      -4.402907     2.671120    -1.666941      25.06
 H      -4.760073     2.659521     0.472763      22.90
 H      -4.200641     3.956518    -0.350869      23.87
 C      -0.839359     1.162497     0.246578      39.70
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 O       0.018585     2.152842     0.888189     186.85
 C      -0.313221    -0.149949     0.237222       5.65
 H       0.841902    -0.096512     0.586127      16.49
 C      -2.430868    -1.146306    -0.658513      40.33
 C      -3.227775    -2.310361    -1.058218      65.23
 H      -4.320810    -1.812402    -1.462803      21.58
 O      -2.566376    -2.919503    -2.383316     249.65
 H      -3.339335    -2.955992    -2.945425      27.28
 C      -3.369130    -3.394063    -0.042844     111.63
 H      -2.342373    -3.614240     0.416928      24.83
 O      -4.092120    -2.586276     0.889291     339.53
 H      -3.532356    -1.955930     1.305595      29.05
 C      -4.293156    -4.617642    -0.370570      94.66
 O      -3.673356    -5.616242    -1.209703     341.13
 H      -2.838737    -6.007003    -0.713838      26.67
 H      -5.107357    -4.329677    -1.010137      26.55
 H      -4.857837    -4.833222     0.516574      26.65
55
name = lig-etoh-frame_104
 C       2.470164     1.410892    -2.142821      53.60
 H       1.692567     1.926427    -2.747257      22.76
 C       3.259940     0.897763     0.086043      79.87
 H       3.397796     1.211390     1.154956      20.46
 C       4.148727    -0.040576    -0.247872      25.41
 O       4.851070    -0.943159     0.521127     217.27
 C       4.965598    -0.687480     2.025973     106.07
 H       4.062954    -0.497620     2.553937      25.83
 H       5.451576     0.302526     2.096552      26.05
 H       5.714162    -1.564008     2.433930      24.10
 C       4.047675    -0.484833    -1.659447      26.15
 O       4.998181    -1.405250    -2.200898     257.63
 H       4.631982    -2.163683    -1.855003      32.71
 C       3.221769     0.256893    -2.563578      45.60
 H       3.012436    -0.490107    -3.393248      20.68
 C       2.723498     1.784576    -0.720932      34.69
 C       2.206396     3.026277    -0.178882      91.38
 H       2.488232     3.860773    -1.094156      20.63
 O       2.709911     3.596156     1.041847     327.17
 H       3.631032     3.578122     0.996965      30.94
 C       0.505727     3.286047    -0.055639      63.83
 H      -0.054747     3.130787    -1.018921      21.50
 C       0.204903     4.637191     0.551961     110.82
 O       0.216431     5.740699    -0.296510     226.45
 H       0.862025     5.587675    -0.993337      33.09
 H       0.794470     4.759747     1.557051      24.63
 H      -0.839006     4.651620     0.979907      25.28
 C      -1.032834    -1.292661    -0.270632      30.06
 H      -0.570625    -2.363518    -0.317869      15.74
 C      -2.941242     0.199851    -0.614748      49.62
 H      -4.123226     0.634623    -0.925930      16.70
 C      -2.224106     1.371600    -0.280457      30.80
 O      -2.658225     2.737324    -0.332372     167.20
 C      -4.246905     2.868824    -0.514695     108.98
 H      -4.641012     2.346200    -1.460283      25.36
 H      -4.889786     2.255494     0.112934      26.39
 H      -3.976779     3.919041    -0.632247      23.98
 C      -0.883485     1.146454     0.255682      13.76
 O       0.056089     2.194878     0.877179     144.15
 C      -0.332009    -0.155664     0.193059      30.76
 H       0.715372    -0.156936     0.535954      17.55
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 C      -2.356113    -1.109601    -0.638888      41.90
 C      -3.226994    -2.324092    -1.153089      71.72
 H      -4.144936    -1.971965    -1.265627      28.71
 O      -2.559570    -2.896552    -2.365945     255.34
 H      -3.334861    -3.041859    -3.123129      24.47
 C      -3.329373    -3.437713    -0.079584      88.13
 H      -2.290871    -3.517770     0.191974      26.22
 O      -4.145201    -2.581751     0.913592     258.93
 H      -3.412604    -1.890575     1.268115      22.47
 C      -4.242514    -4.620914    -0.470530      75.87
 O      -3.722563    -5.610569    -1.177909     359.29
 H      -2.787007    -5.982898    -0.936757      27.83
 H      -4.947278    -3.947817    -1.126146      24.10
 H      -4.752836    -5.006585     0.551165      22.64
55
name = lig-etoh-frame_105
 C       2.539959     1.394319    -2.106411      33.51
 H       1.699139     1.884890    -2.572551      21.82
 C       3.197644     0.841658     0.181409      89.92
 H       3.373024     1.438722     1.101918      20.66
 C       4.204959    -0.113875    -0.327953      20.72
 O       4.852016    -0.884475     0.525616     211.21
 C       4.962318    -0.702725     2.006456     107.63
 H       3.936634    -0.559975     2.499193      23.96
 H       5.527588     0.260593     2.207419      25.49
 H       5.636435    -1.443980     2.388903      25.92
 C       4.025990    -0.465127    -1.619920      33.58
 O       4.978197    -1.337928    -2.238087     178.58
 H       4.688379    -2.413811    -1.916311      24.40
 C       3.201592     0.142980    -2.552577      26.44
 H       3.065547    -0.447166    -3.426242      21.38
 C       2.691661     1.755309    -0.769011      21.73
 C       2.156842     3.077737    -0.197538     110.57
 H       2.447881     3.653151    -0.949736      25.02
 O       2.686127     3.621109     1.075929     318.39
 H       3.737385     3.560353     1.086825      28.68
 C       0.621015     3.264152    -0.092006      73.54
 H      -0.006068     3.168766    -0.956378      22.33
 C       0.210665     4.558634     0.608639     101.29
 O       0.213090     5.755682    -0.303691     146.90
 H       0.822895     5.705789    -1.208391      28.99
 H       0.891940     4.877744     1.368668      25.06
 H      -0.858453     4.498994     0.804298      25.24
 C      -1.010127    -1.226023    -0.280003      43.26
 H      -0.762747    -2.187354     0.122206      16.93
 C      -3.007478     0.162869    -0.628178      57.77
 H      -3.901838     0.457337    -0.880324      19.26
 C      -2.202198     1.351786    -0.326742      10.84
 O      -2.641415     2.662916    -0.331333     180.37
 C      -4.195078     2.909498    -0.473255     106.08
 H      -4.570270     2.321862    -1.338720      25.27
 H      -4.830437     2.206755     0.189255      24.12
 H      -4.393542     3.986178    -0.779291      24.64
 C      -0.898619     1.155891     0.266495       8.09
 O       0.053809     2.214611     0.842128     145.36
 C      -0.351460    -0.138593     0.151114      36.21
 H       0.817163    -0.398881     0.572500      14.96
 C      -2.331042    -1.073287    -0.649938      25.22
 C      -3.170788    -2.339590    -1.247082      51.50
 H      -4.396832    -2.029203    -1.338643      22.41
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 O      -2.570080    -2.865977    -2.368930     306.58
 H      -3.145283    -3.158840    -3.043374      26.62
 C      -3.305264    -3.408619    -0.103376      80.90
 H      -2.241982    -3.779967     0.230553      20.30
 O      -4.169342    -2.597093     0.941898     254.60
 H      -3.472032    -2.027332     1.298692      26.03
 C      -4.221560    -4.547398    -0.508572     103.54
 O      -3.751601    -5.651363    -1.217756     393.84
 H      -2.955055    -5.905651    -0.793737      33.74
 H      -4.929694    -4.015245    -1.096609      28.08
 H      -4.632452    -5.000896     0.338896      25.37
55
name = lig-etoh-frame_106
 C       2.606228     1.325894    -2.094098      53.59
 H       1.847412     1.872683    -2.725937      17.47
 C       3.217401     0.825666     0.266296      59.52
 H       3.322823     1.323475     1.219345      19.75
 C       4.154809    -0.137644    -0.317515       4.46
 O       4.902607    -0.876069     0.565907     218.76
 C       4.949517    -0.655034     1.954799     112.66
 H       3.927826    -0.851571     2.392510      24.32
 H       5.508537     0.209396     2.267030      26.06
 H       5.533887    -1.608267     2.366122      23.99
 C       4.060619    -0.481293    -1.662090      36.07
 O       4.941525    -1.316633    -2.261568     274.53
 H       5.041191    -2.230098    -2.109746      27.45
 C       3.130783     0.092208    -2.511250      36.32
 H       3.087127    -0.172056    -3.645361      25.00
 C       2.629575     1.711807    -0.772600      42.18
 C       2.101145     3.145843    -0.221451      92.49
 H       2.514957     3.955584    -1.092540      22.47
 O       2.666305     3.613011     1.102530     275.76
 H       3.677288     3.779701     1.072648      28.56
 C       0.699466     3.213415    -0.093936      82.02
 H       0.227506     3.249611    -1.159129      19.48
 C       0.210098     4.521865     0.621145      89.20
 O       0.216755     5.781201    -0.330354     176.53
 H       0.551484     5.554256    -1.180088      33.72
 H       0.919433     4.849591     1.407079      23.57
 H      -0.846461     4.286600     0.850512      23.65
 C      -1.020262    -1.205465    -0.274717      43.83
 H      -0.736280    -2.113543     0.301852      17.23
 C      -2.990878     0.175253    -0.638221      38.05
 H      -4.236899     0.132447    -1.050242      15.57
 C      -2.172691     1.324705    -0.325899      17.17
 O      -2.671928     2.601769    -0.333394     213.35
 C      -4.123594     2.893155    -0.466580     103.34
 H      -4.291618     2.448908    -1.476209      23.44
 H      -4.516192     2.694711     0.578691      23.82
 H      -4.724657     3.830244    -0.555589      24.76
 C      -0.858022     1.195362     0.255597       5.72
 O       0.017435     2.198220     0.794124     180.24
 C      -0.293465    -0.087484     0.157159      41.46
 H       0.606710    -0.328883     0.533087      17.22
 C      -2.393692    -1.071711    -0.721330      32.95
 C      -3.156547    -2.318823    -1.254877      85.70
 H      -4.067580    -2.083942    -1.564121      24.91
 O      -2.547422    -2.840340    -2.407226     294.37
 H      -3.172346    -3.342706    -2.960793      24.37
 C      -3.286758    -3.346252    -0.110487     100.34
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 H      -2.496162    -3.884947     0.360150      20.91
 O      -4.155016    -2.648143     0.949919     276.70
 H      -3.530737    -2.080242     1.470663      25.69
 C      -4.228554    -4.459524    -0.527576      84.13
 O      -3.766209    -5.696422    -1.309584     267.30
 H      -3.074100    -6.096328    -0.515720      23.15
 H      -5.199075    -4.200236    -1.140022      25.95
 H      -4.776801    -4.866898     0.485001      24.35
55
name = lig-etoh-frame_107
 C       2.604579     1.274783    -2.098707      55.11
 H       2.229486     1.846517    -2.948081      18.39
 C       3.268359     0.862994     0.264403      45.86
 H       3.275608     0.992730     1.406742      18.16
 C       4.041008    -0.130857    -0.210169       2.65
 O       4.984892    -0.894600     0.574417     227.70
 C       4.938284    -0.655116     1.926031     123.78
 H       3.927481    -0.853755     2.346739      26.03
 H       5.390521     0.321204     2.357923      25.58
 H       5.399724    -1.605967     2.283286      25.46
 C       4.089447    -0.533107    -1.718078       8.58
 O       4.948470    -1.306796    -2.316880     224.26
 H       5.231293    -2.242363    -2.035186      23.39
 C       3.065313     0.078211    -2.506654      61.46
 H       3.130482     0.068205    -3.543786      26.41
 C       2.582493     1.677771    -0.678115      47.89
 C       2.167899     3.204327    -0.267149     107.91
 H       2.341988     3.980760    -0.872840      26.56
 O       2.649262     3.585581     1.111478     279.60
 H       3.529515     3.981195     0.985318      28.70
 C       0.656289     3.203136    -0.100854      80.41
 H       0.436084     3.170012    -1.127785      20.82
 C       0.204761     4.527985     0.575606      89.92
 O       0.210517     5.780707    -0.334218     198.22
 H       0.293136     5.314401    -1.273913      27.28
 H       0.770053     4.702583     1.538673      23.06
 H      -0.782361     4.265103     1.013363      23.27
 C      -1.067274    -1.197937    -0.247995      52.81
 H      -0.632122    -2.169495     0.089039      16.33
 C      -2.997607     0.199110    -0.688161      48.05
 H      -3.942752     0.035382    -0.985000      15.84
 C      -2.182767     1.308659    -0.292255      12.88
 O      -2.694282     2.601929    -0.334443     229.88
 C      -4.062158     2.840242    -0.442367     110.27
 H      -4.419943     2.329287    -1.381563      24.07
 H      -4.353585     2.760212     0.615741      24.57
 H      -4.272452     3.972429    -0.422451      24.67
 C      -0.788930     1.229450     0.202262      20.38
 O      -0.026078     2.173234     0.738697     210.63
 C      -0.271737    -0.043792     0.159973      34.83
 H       0.906337    -0.186796     0.758468      14.79
 C      -2.421816    -1.092158    -0.797691      49.20
 C      -3.113473    -2.279956    -1.210306      62.17
 H      -4.220352    -1.923562    -1.705732      21.12
 O      -2.492420    -2.823198    -2.486625     176.60
 H      -3.207194    -3.648793    -2.674426      20.27
 C      -3.335938    -3.284870    -0.105105      98.75
 H      -2.459129    -3.804323     0.463404      20.69
 O      -4.115982    -2.708757     0.942988     304.58
 H      -3.560815    -2.138656     1.636149      24.94
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 C      -4.319214    -4.447922    -0.549345      97.60
 O      -3.763654    -5.709127    -1.362795     287.93
 H      -3.364936    -6.332391    -0.776976      29.06
 H      -5.184013    -4.215083    -1.114992      30.66
 H      -4.678752    -4.645697     0.389797      28.59
55
name = lig-etoh-frame_108
 C       2.542057     1.301788    -2.033956      54.23
 H       2.518867     1.991521    -2.929024      18.12
 C       3.300747     0.927067     0.277584      53.38
 H       3.182322     0.870933     1.306537      20.24
 C       3.989907    -0.211835    -0.184836       2.23
 O       5.049562    -0.896994     0.530538     217.04
 C       4.922761    -0.685245     1.960147     111.94
 H       3.821717    -0.641025     2.304789      25.69
 H       5.253425     0.270637     2.293798      27.46
 H       5.542391    -1.535090     2.428613      25.48
 C       4.041960    -0.550950    -1.681279      -6.82
 O       4.998486    -1.335862    -2.408881     146.59
 H       5.350673    -2.112166    -1.645558      21.87
 C       3.075862     0.042726    -2.509086      22.07
 H       3.183408    -0.021339    -3.658239      21.59
 C       2.555773     1.701716    -0.628425      49.44
 C       2.235227     3.177294    -0.223932      97.26
 H       2.397252     4.133527    -1.012576      21.94
 O       2.642073     3.543271     1.098516     265.09
 H       3.502164     4.186364     1.000333      25.52
 C       0.580141     3.235098    -0.110372      67.74
 H       0.205813     2.988388    -1.201774      18.44
 C       0.167159     4.554064     0.534859     103.16
 O       0.209218     5.727413    -0.330127     222.54
 H      -0.071925     5.342995    -1.283757      27.05
 H       0.754358     4.686122     1.420014      24.90
 H      -0.854663     4.455301     0.935346      24.19
 C      -1.095530    -1.180745    -0.216365      51.78
 H      -0.664644    -2.177793    -0.328482      15.20
 C      -2.942095     0.204461    -0.742896      53.18
 H      -4.201435     0.344213    -1.045717      18.66
 C      -2.208721     1.319854    -0.251130      32.00
 O      -2.659643     2.616888    -0.337038     248.22
 C      -4.028399     2.832591    -0.392122     118.33
 H      -4.765135     2.255698    -1.048716      24.70
 H      -4.621788     2.372687     0.513520      25.74
 H      -3.648430     3.891100    -0.605182      21.01
 C      -0.777466     1.211173     0.095874      36.72
 O      -0.039363     2.190363     0.695506     220.92
 C      -0.238162    -0.072938     0.184349      30.26
 H       0.609994    -0.078514     0.602530      20.70
 C      -2.340493    -1.065482    -0.815298      44.80
 C      -3.121347    -2.235755    -1.234363      83.96
 H      -4.044940    -1.902576    -1.410849      27.50
 O      -2.466966    -2.834774    -2.544943     255.88
 H      -2.765279    -3.703947    -2.471526      25.15
 C      -3.393185    -3.280727    -0.097760      90.26
 H      -2.404948    -3.575650     0.179265      26.33
 O      -4.091594    -2.746507     0.957372     364.63
 H      -3.487609    -2.269610     1.490466      29.78
 C      -4.378213    -4.497002    -0.592338      62.67
 O      -3.799589    -5.666085    -1.413255     278.98
 H      -3.391457    -6.407527    -0.853628      27.28
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 H      -5.203789    -4.015801    -1.256382      27.26
 H      -4.711569    -4.822335     0.541818      24.65
55
name = lig-etoh-frame_109
 C       2.486163     1.341101    -1.958558      60.28
 H       2.474478     2.196828    -2.631878      18.97
 C       3.320859     0.935450     0.281877      69.45
 H       3.111047     1.124405     1.410270      17.86
 C       4.005863    -0.324603    -0.245231       8.60
 O       5.078929    -0.887518     0.485837     190.86
 C       4.897478    -0.726071     2.004013      98.66
 H       3.877964    -0.706366     2.245462      27.61
 H       5.317526     0.345075     2.172000      25.00
 H       5.632515    -1.352378     2.662188      25.12
 C       3.980899    -0.574352    -1.623935       2.94
 O       5.043753    -1.382458    -2.436604     207.73
 H       5.405543    -1.739985    -1.737293      28.98
 C       3.115117     0.055609    -2.507091       9.13
 H       3.182415    -0.260283    -3.529750      21.17
 C       2.566774     1.765971    -0.643388      47.62
 C       2.215993     3.151220    -0.180565     117.64
 H       2.588099     3.738711    -0.937908      23.09
 O       2.660636     3.512987     1.085319     330.76
 H       3.428040     4.045594     1.133354      30.63
 C       0.512464     3.263426    -0.166518      77.05
 H       0.008915     3.107004    -1.061214      22.09
 C       0.086849     4.582777     0.501600     106.93
 O       0.202340     5.662792    -0.341259     262.16
 H      -0.165443     5.552764    -1.144609      33.91
 H       0.906218     4.816222     1.295264      24.30
 H      -0.994775     4.580778     0.779625      24.62
 C      -1.049154    -1.181128    -0.202390      50.33
 H      -0.654247    -2.152161    -0.616048      16.66
 C      -2.924899     0.233228    -0.796576      60.34
 H      -3.839011     0.663551    -1.013305      23.22
 C      -2.192696     1.322618    -0.237853      23.46
 O      -2.587136     2.594489    -0.333537     229.34
 C      -4.045514     2.847045    -0.324910     124.08
 H      -4.721285     2.402979    -1.113468      26.90
 H      -4.606678     2.481116     0.523707      27.69
 H      -4.021962     3.888022    -0.706614      25.57
 C      -0.814071     1.157664    -0.002978      39.92
 O      -0.036321     2.225725     0.672067     190.82
 C      -0.294066    -0.127961     0.175499      22.15
 H       0.954884    -0.203272     0.652836      15.34
 C      -2.262208    -1.002455    -0.800951      33.95
 C      -3.123138    -2.215669    -1.290332      49.85
 H      -4.277661    -1.753379    -1.451373      21.88
 O      -2.470843    -2.838968    -2.551675     222.90
 H      -2.343521    -3.896739    -2.431355      20.44
 C      -3.418580    -3.331492    -0.156212      80.81
 H      -2.305855    -3.636512    -0.018076      22.58
 O      -4.086734    -2.765284     0.991336     327.65
 H      -3.312685    -2.224519     1.428191      23.36
 C      -4.403037    -4.568717    -0.610300     100.61
 O      -3.859839    -5.589152    -1.460544     323.07
 H      -3.286368    -6.145783    -0.770181      27.32
 H      -5.102374    -3.999431    -1.207888      28.49
 H      -4.840666    -5.046280     0.169442      27.76
55
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name = lig-etoh-frame_110
 C       2.469211     1.353268    -1.946477      50.31
 H       2.104608     2.234365    -2.556495      22.69
 C       3.317981     0.883977     0.266007      47.02
 H       3.321406     1.353903     1.219709      19.15
 C       4.034062    -0.355719    -0.260891      16.64
 O       5.090917    -0.898042     0.471708     201.61
 C       4.923038    -0.711860     2.015546     103.02
 H       3.789035    -0.964805     2.301643      24.55
 H       5.235086     0.280384     2.114797      26.60
 H       5.534539    -1.355572     2.614766      26.46
 C       3.958629    -0.636211    -1.636038      14.80
 O       5.035779    -1.398811    -2.421782     151.89
 H       5.795053    -1.705115    -1.637799      22.95
 C       3.126422     0.150491    -2.455482      65.79
 H       3.107063    -0.307544    -3.477394      19.88
 C       2.634752     1.768642    -0.617617      25.19
 C       2.123946     3.115401    -0.169312      94.65
 H       2.770560     3.722243    -1.037519      18.65
 O       2.665035     3.476936     1.105893     296.38
 H       3.630906     3.907386     1.092695      26.73
 C       0.468790     3.292270    -0.199933      71.89
 H      -0.038517     3.356615    -1.270551      19.56
 C       0.009062     4.592932     0.488068     111.86
 O       0.215088     5.659061    -0.369751     204.03
 H      -0.283270     5.641645    -1.304913      28.31
 H       0.683383     4.829528     1.251657      26.64
 H      -1.012749     4.454765     0.866166      25.68
 C      -0.974597    -1.250426    -0.248330      61.38
 H      -0.466829    -2.156782    -0.478781      17.83
 C      -2.866514     0.297650    -0.810626      54.72
 H      -3.962476     0.622363    -1.237258      20.67
 C      -2.137343     1.299164    -0.272214      24.50
 O      -2.552917     2.600046    -0.321159     216.78
 C      -4.075452     2.882842    -0.303540     103.12
 H      -4.393019     2.427399    -1.305790      23.98
 H      -4.406074     2.827849     0.829895      23.65
 H      -4.576376     3.925145    -0.455157      25.09
 C      -0.806654     1.125920    -0.014172      50.85
 O      -0.045826     2.229298     0.647924     190.80
 C      -0.266737    -0.151316     0.190234      24.82
 H       0.609994    -0.330441     0.411025      21.67
 C      -2.288953    -0.970235    -0.803351      34.83
 C      -3.160787    -2.202435    -1.352454      71.91
 H      -4.008847    -1.819176    -1.756290      24.21
 O      -2.507693    -2.846639    -2.519414     254.80
 H      -2.033297    -3.760830    -2.345872      23.54
 C      -3.414108    -3.407474    -0.242164      80.88
 H      -2.493399    -3.883372     0.052443      24.10
 O      -4.055717    -2.778743     1.022556     296.65
 H      -3.351333    -2.129758     1.409678      23.10
 C      -4.403555    -4.585610    -0.648064      94.89
 O      -3.892174    -5.520557    -1.497270     335.47
 H      -3.214264    -5.868599    -0.965972      33.72
 H      -5.239879    -4.068761    -1.220802      25.56
 H      -5.107695    -5.212964     0.154718      23.63
55
name = lig-etoh-frame_111
 C       2.474129     1.365292    -1.977043      23.29
 H       1.689805     1.830961    -2.630947      20.71
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 C       3.326406     0.809721     0.217807      62.22
 H       3.705086     1.301712     1.180706      19.84
 C       4.058520    -0.309272    -0.238152       8.20
 O       5.094752    -0.930236     0.496224     201.20
 C       4.924642    -0.700459     1.977828     103.36
 H       4.005669    -1.006789     2.289235      27.76
 H       5.093994     0.403853     2.281775      24.04
 H       5.644813    -1.574168     2.433885      24.23
 C       3.989115    -0.700617    -1.674116      11.55
 O       4.995734    -1.406126    -2.349129     204.63
 H       5.901276    -1.580025    -1.881169      24.71
 C       3.118793     0.258774    -2.406952      67.38
 H       2.940054    -0.026709    -3.469221      23.64
 C       2.699062     1.703392    -0.580695      33.02
 C       2.056060     3.106817    -0.209737     101.24
 H       2.464631     3.839194    -0.837557      23.16
 O       2.662633     3.452236     1.150103     292.66
 H       3.631029     3.619389     0.874000      27.63
 C       0.447013     3.317124    -0.225386      84.87
 H       0.199291     3.392496    -1.238191      21.60
 C      -0.059312     4.576159     0.478109      98.53
 O       0.221582     5.714498    -0.422683     205.56
 H      -0.256847     5.528712    -1.326827      28.85
 H       0.497742     4.788286     1.492914      23.79
 H      -1.065363     4.323808     0.919559      23.45
 C      -0.952169    -1.314564    -0.340208      61.36
 H      -0.359223    -2.291296    -0.177081      19.47
 C      -2.856333     0.324097    -0.834748      55.82
 H      -3.812158     0.167992    -1.401556      22.36
 C      -2.089900     1.336848    -0.334448       4.71
 O      -2.553491     2.673450    -0.300446     211.23
 C      -4.091503     2.931158    -0.277300     105.06
 H      -4.321438     2.208361    -1.101657      24.82
 H      -4.284766     2.673232     0.719984      27.12
 H      -4.410776     3.976141    -0.256932      25.67
 C      -0.725107     1.130478     0.068756      36.61
 O      -0.072464     2.202814     0.604092     201.46
 C      -0.259939    -0.168326     0.171690      13.53
 H       1.022639    -0.395434     0.447664      14.71
 C      -2.337938    -1.026817    -0.812223      30.66
 C      -3.148184    -2.230471    -1.385939      53.73
 H      -4.112795    -1.823608    -2.062074      19.16
 O      -2.538208    -2.851042    -2.485811     286.58
 H      -2.051621    -3.523691    -2.147969      26.78
 C      -3.448748    -3.450706    -0.282913      70.79
 H      -2.553762    -4.055331     0.111651      19.41
 O      -4.006796    -2.801929     1.021592     313.80
 H      -3.440036    -2.139979     1.379635      24.85
 C      -4.490885    -4.545739    -0.671556      98.89
 O      -3.888818    -5.480656    -1.558394     327.43
 H      -2.975971    -5.890156    -1.216803      28.69
 H      -5.359376    -4.151915    -1.237054      26.34
 H      -4.889503    -4.923050     0.200332      27.96
55
name = lig-etoh-frame_112
 C       2.457304     1.382710    -1.965598      40.76
 H       1.561319     1.460591    -2.581423      20.41
 C       3.386109     0.760218     0.221711      71.42
 H       3.903950     1.030773     1.124920      23.31
 C       4.107759    -0.293090    -0.282070      14.33
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 O       5.076140    -0.951472     0.542848     214.62
 C       4.972050    -0.717952     1.924808     123.02
 H       3.872699    -1.056732     2.305991      24.41
 H       5.073726     0.232548     2.424789      26.31
 H       5.700725    -1.350511     2.229427      27.70
 C       4.028578    -0.672879    -1.658243      18.62
 O       4.937569    -1.417761    -2.292579     249.48
 H       5.730349    -1.448665    -1.872748      27.65
 C       3.144683     0.272973    -2.421458      71.36
 H       2.894435     0.227516    -3.474570      24.84
 C       2.670416     1.686080    -0.617102      53.71
 C       2.015112     3.093805    -0.191364      99.62
 H       2.242829     4.082258    -0.903862      21.37
 O       2.638897     3.421675     1.172720     300.75
 H       3.535373     3.517634     0.927290      29.90
 C       0.480122     3.307376    -0.204369      74.82
 H       0.214583     3.202749    -1.342232      20.81
 C      -0.098546     4.568054     0.491278     103.70
 O       0.203435     5.765793    -0.455926     226.08
 H      -0.067702     5.476532    -1.269245      33.54
 H       0.370810     4.736051     1.403990      26.47
 H      -1.184175     4.405722     0.615289      23.98
 C      -0.964911    -1.336663    -0.417611      64.89
 H      -0.642566    -2.287070    -0.029729      21.69
 C      -2.841420     0.235158    -0.876532      37.21
 H      -3.831055     0.191834    -1.436983      20.36
 C      -2.062077     1.430615    -0.402559     -14.44
 O      -2.553877     2.774294    -0.278905     192.08
 C      -4.047966     2.931514    -0.234183      93.87
 H      -4.659502     2.219545    -0.866644      24.65
 H      -4.419872     2.237833     0.695058      23.75
 H      -4.021784     4.066585    -0.380047      23.78
 C      -0.683796     1.134875     0.156134       4.86
 O      -0.083320     2.190209     0.568304     200.21
 C      -0.179881    -0.231654     0.129824      29.89
 H       0.734154    -0.221211     0.469615      19.60
 C      -2.332983    -1.124797    -0.811449      26.23
 C      -3.174958    -2.257663    -1.401708      78.96
 H      -4.100308    -1.912925    -1.717440      23.42
 O      -2.544826    -2.864895    -2.480651     222.74
 H      -1.932607    -3.558999    -1.940501      20.86
 C      -3.513573    -3.429793    -0.269449      66.84
 H      -2.582660    -3.974944    -0.106867      20.60
 O      -3.968397    -2.852085     0.983346     276.31
 H      -3.304444    -2.083820     1.338758      19.84
 C      -4.566607    -4.475253    -0.706181      70.54
 O      -3.871554    -5.464200    -1.634748     313.76
 H      -3.004273    -5.850620    -1.314556      28.94
 H      -5.440515    -4.135609    -1.270512      26.28
 H      -4.702471    -4.822385     0.477113      23.78
55
name = lig-etoh-frame_113
 C       2.432906     1.341834    -1.931369      59.27
 H       1.500457     1.593230    -2.512552      17.38
 C       3.453901     0.779466     0.225008      73.08
 H       3.774831     1.028743     1.251352      21.23
 C       4.175438    -0.314941    -0.340472      12.71
 O       5.045165    -0.957056     0.548226     235.70
 C       4.972812    -0.766910     1.911242     115.03
 H       4.072147    -1.117620     2.274188      26.94
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 H       5.204496     0.274775     2.342878      25.13
 H       5.992374    -1.325558     2.380931      23.74
 C       4.033186    -0.541193    -1.651362      27.52
 O       4.873924    -1.458867    -2.271731     158.94
 H       5.791373    -1.366138    -1.585334      22.17
 C       3.200908     0.222155    -2.464749      60.72
 H       3.096393     0.106386    -3.601386      25.49
 C       2.589325     1.724642    -0.636556      74.67
 C       2.025331     3.116209    -0.135260     124.85
 H       2.259892     3.855493    -0.859610      26.82
 O       2.576251     3.384502     1.172806     289.51
 H       3.627165     3.615495     1.133955      27.32
 C       0.520512     3.248872    -0.183060      81.54
 H       0.114874     3.060431    -1.155477      23.70
 C      -0.128486     4.581699     0.435878      96.97
 O       0.171996     5.798200    -0.439139     185.13
 H       0.213306     5.410485    -1.485960      25.65
 H       0.378482     4.791851     1.453036      24.41
 H      -1.217832     4.551100     0.277559      23.07
 C      -0.981961    -1.324066    -0.435265      50.64
 H      -0.853078    -2.397115    -0.122077      18.18
 C      -2.802450     0.147305    -0.913499      30.86
 H      -3.842272     0.579681    -1.294119      20.48
 C      -2.045941     1.455143    -0.461580     -19.45
 O      -2.552461     2.830701    -0.274290     192.09
 C      -3.990593     2.869743    -0.165182     122.11
 H      -4.802880     2.658093    -0.993747      25.18
 H      -4.412126     2.484447     0.696323      28.45
 H      -4.011235     3.969751    -0.356029      25.42
 C      -0.758389     1.084958     0.153733      -6.53
 O      -0.050357     2.214182     0.590880     201.19
 C      -0.171828    -0.258787     0.054222      34.07
 H       0.987881    -0.313395     0.661325      15.06
 C      -2.302036    -1.179126    -0.819955      26.88
 C      -3.218211    -2.292428    -1.339898      69.43
 H      -4.335282    -1.829784    -1.493202      22.11
 O      -2.523979    -2.906845    -2.485315     214.68
 H      -1.885123    -3.600797    -2.097910      23.43
 C      -3.570214    -3.350419    -0.280470      78.27
 H      -2.559283    -3.912108    -0.310932      20.36
 O      -3.929053    -2.893775     0.943063     339.84
 H      -3.274558    -2.251972     1.223212      26.03
 C      -4.570352    -4.438885    -0.706466      91.39
 O      -3.883242    -5.437511    -1.704089     302.06
 H      -3.162479    -5.759417    -1.158982      29.55
 H      -5.536279    -4.110176    -1.214226      26.42
 H      -4.801152    -4.937165     0.162167      28.06
55
name = lig-etoh-frame_114
 C       2.393832     1.244515    -1.940793      62.19
 H       1.721338     1.926569    -2.492709      19.75
 C       3.496615     0.870123     0.195706      84.85
 H       3.389961     1.154500     1.286715      18.69
 C       4.197117    -0.255194    -0.283715      14.50
 O       5.034462    -0.986590     0.496313     226.36
 C       5.041370    -0.807760     1.959684     117.52
 H       4.071114    -1.284189     2.465444      25.88
 H       5.185777     0.273043     2.040074      26.16
 H       5.790164    -1.303123     2.365515      29.33
 C       4.063606    -0.435641    -1.722951      31.48
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 O       4.844373    -1.504684    -2.238672     211.03
 H       5.589634    -1.583153    -1.634291      24.28
 C       3.214078     0.209003    -2.529308      24.02
 H       3.377642    -0.164764    -3.508655      23.47
 C       2.549980     1.737148    -0.583168      73.48
 C       2.073581     3.110739    -0.080004     110.99
 H       2.593839     3.841121    -0.931508      20.98
 O       2.518173     3.357779     1.185167     303.94
 H       3.389006     3.772918     1.255432      30.67
 C       0.520236     3.193842    -0.143596      85.12
 H       0.120682     3.087880    -1.206876      21.12
 C      -0.125013     4.616774     0.324064     109.35
 O       0.144794     5.803838    -0.438412     280.65
 H       0.624037     5.606494    -1.265672      31.17
 H       0.126832     4.819588     1.357631      26.14
 H      -1.210821     4.495033     0.286684      24.96
 C      -0.973919    -1.338554    -0.394192      45.68
 H      -0.668690    -2.406370    -0.370271      17.63
 C      -2.769481     0.190459    -0.929206      49.64
 H      -3.736523     0.488368    -1.165615      21.06
 C      -2.029973     1.370308    -0.494223       7.98
 O      -2.540904     2.799802    -0.294821     184.59
 C      -3.969239     2.871899    -0.137229     118.26
 H      -4.445678     2.796728    -1.130674      24.08
 H      -4.352921     2.727250     1.002955      23.13
 H      -4.256571     3.987149    -0.019587      25.66
 C      -0.840091     1.068259     0.083354      -0.47
 O      -0.018947     2.195774     0.677689     183.08
 C      -0.170652    -0.244475     0.006242      57.06
 H       0.682660    -0.553626     0.503726      19.63
 C      -2.315699    -1.156292    -0.857442      25.49
 C      -3.276665    -2.300975    -1.271507      81.73
 H      -4.145230    -1.787995    -1.647041      24.84
 O      -2.521729    -2.942768    -2.490096     228.63
 H      -2.023051    -3.664124    -2.242051      27.39
 C      -3.566757    -3.326336    -0.343111     100.28
 H      -2.644035    -3.909773    -0.262091      22.50
 O      -3.907882    -2.920033     0.935183     354.34
 H      -3.239824    -2.282932     1.300930      27.66
 C      -4.555022    -4.437146    -0.759955      91.51
 O      -3.917105    -5.384725    -1.745218     271.76
 H      -3.321701    -5.823389    -0.975625      26.09
 H      -5.468816    -4.048403    -1.153128      26.94
 H      -5.017492    -5.222080     0.077898      24.57
55
name = lig-etoh-frame_115
 C       2.347072     1.196135    -1.951013      62.13
 H       2.067757     2.045972    -2.642057      21.79
 C       3.480626     1.007878     0.192105      59.76
 H       3.256029     1.187813     1.208566      20.62
 C       4.170636    -0.122795    -0.231104       4.86
 O       5.041803    -1.052721     0.443296     196.45
 C       5.068797    -0.826884     1.980880     101.38
 H       4.209375    -1.185058     2.522889      27.52
 H       5.087597     0.265434     2.038944      25.77
 H       6.020752    -1.528926     2.387640      24.39
 C       4.163569    -0.411694    -1.729077       8.57
 O       4.808255    -1.546479    -2.218094     197.13
 H       5.527490    -1.853657    -1.611907      23.93
 C       3.188865     0.236071    -2.588848      51.25
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 H       3.368371    -0.256023    -3.620692      22.77
 C       2.575046     1.658755    -0.567013      44.61
 C       2.125659     3.093951    -0.103686     113.69
 H       2.723684     3.763929    -0.684690      23.64
 O       2.460966     3.348411     1.251483     296.78
 H       3.278235     3.900218     1.221612      28.19
 C       0.500289     3.197548    -0.135596      78.45
 H       0.301578     3.086634    -1.213246      21.99
 C      -0.129708     4.622838     0.218541     113.85
 O       0.141932     5.821079    -0.445666     277.91
 H       0.851783     5.708495    -1.124654      30.71
 H       0.004422     4.830532     1.344637      24.66
 H      -1.198759     4.331138     0.310138      24.33
 C      -0.979145    -1.368064    -0.365366      43.52
 H      -0.345236    -2.261145    -0.520163      15.99
 C      -2.752366     0.267941    -0.936926      51.58
 H      -3.960981     0.199710    -1.185634      21.14
 C      -2.059724     1.295089    -0.503819      20.26
 O      -2.514222     2.706781    -0.326584     205.81
 C      -3.966406     2.951273    -0.087170     110.46
 H      -4.287013     2.484344    -1.102445      23.33
 H      -4.263473     2.422778     0.807250      27.18
 H      -4.221416     3.989166     0.166269      26.15
 C      -0.791065     1.086870     0.028737       8.75
 O      -0.018405     2.121676     0.781600     164.72
 C      -0.250954    -0.223208    -0.038743      47.32
 H       0.815110    -0.571961     0.490396      17.44
 C      -2.332892    -1.095168    -0.884750      33.16
 C      -3.259487    -2.248866    -1.304612      67.38
 H      -4.134393    -1.774058    -1.947010      23.14
 O      -2.554179    -2.943438    -2.489293     167.09
 H      -2.267088    -3.970321    -2.210560      21.40
 C      -3.536507    -3.410420    -0.351797      80.78
 H      -2.570325    -3.971624    -0.170063      24.31
 O      -3.911878    -2.927467     0.961707     347.81
 H      -3.247045    -2.258973     1.453426      24.69
 C      -4.571416    -4.481121    -0.827087      97.89
 O      -3.947814    -5.325646    -1.745132     306.16
 H      -3.491021    -6.026882    -1.266480      32.37
 H      -5.443977    -3.885432    -1.311480      26.85
 H      -4.938939    -5.039370    -0.017705      28.11
55
name = lig-etoh-frame_116
 C       2.341084     1.216953    -1.977493      65.51
 H       2.102378     1.920523    -2.749449      24.07
 C       3.470236     1.094109     0.258337      48.38
 H       3.424069     1.289887     1.386188      19.03
 C       4.177293    -0.031938    -0.268709       4.69
 O       5.027964    -1.100791     0.425722     177.50
 C       5.128668    -0.860650     1.960850     113.79
 H       4.156149    -1.184548     2.494818      26.18
 H       5.204540     0.219466     2.278360      27.01
 H       5.978958    -1.326063     2.215161      29.19
 C       4.231265    -0.402658    -1.673618       3.16
 O       4.774735    -1.572124    -2.208342     147.68
 H       5.410088    -2.191452    -1.480147      20.90
 C       3.210577     0.225949    -2.598671      61.19
 H       3.006523     0.035054    -3.645443      21.70
 C       2.577105     1.602304    -0.652580      57.06
 C       2.121782     3.040346    -0.114789     110.23
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 H       2.723063     3.902070    -0.730957      22.33
 O       2.418771     3.348100     1.343976     244.18
 H       3.280095     3.954859     1.249658      25.60
 C       0.526734     3.235211    -0.157451      52.12
 H       0.271175     2.897192    -1.185377      21.12
 C      -0.156471     4.573853     0.201959     105.58
 O       0.147985     5.852721    -0.468839     222.97
 H       0.986640     5.699169    -1.151862      27.15
 H       0.096680     4.764078     1.251148      24.77
 H      -1.227099     4.345496     0.034557      24.08
 C      -1.020896    -1.368614    -0.388295      63.24
 H      -0.290364    -2.194173    -0.577945      17.99
 C      -2.850591     0.233471    -0.973251      59.96
 H      -3.801145     0.265333    -1.197253      27.10
 C      -2.080827     1.350606    -0.459897       1.02
 O      -2.476581     2.600287    -0.354670     195.10
 C      -3.939104     2.960036    -0.068419     104.61
 H      -4.568530     2.465675    -0.802604      26.14
 H      -4.273074     1.995201     0.624686      23.45
 H      -4.006575     4.041828     0.017978      25.30
 C      -0.676136     1.113098     0.011235      21.21
 O      -0.035820     2.040627     0.839821     132.26
 C      -0.300049    -0.215803    -0.031489      42.57
 H       0.795751    -0.172792     0.263624      18.91
 C      -2.309816    -1.062458    -0.888229      35.58
 C      -3.203141    -2.193981    -1.418282      69.94
 H      -4.175483    -1.906266    -1.898915      23.97
 O      -2.580255    -2.952978    -2.479848     246.02
 H      -2.793250    -3.888202    -2.274170      22.83
 C      -3.491165    -3.487719    -0.294792      67.88
 H      -2.512339    -3.983786    -0.225847      24.39
 O      -3.937388    -2.933157     1.001131     349.34
 H      -3.321609    -2.345622     1.370621      28.11
 C      -4.596566    -4.463853    -0.885596      88.99
 O      -3.969306    -5.300277    -1.776029     305.46
 H      -3.634556    -6.154220    -1.509500      32.02
 H      -5.310861    -3.934883    -1.460508      27.89
 H      -4.987787    -4.931731     0.175363      25.03
55
name = lig-etoh-frame_117
 C       2.409091     1.235611    -2.041654      48.96
 H       1.734539     1.836992    -2.766669      21.65
 C       3.492342     1.080346     0.333487      32.72
 H       3.669481     1.472526     1.299294      20.81
 C       4.240776    -0.010095    -0.315682      14.80
 O       4.989163    -1.092133     0.445745     181.65
 C       5.152729    -0.866874     1.899667     108.73
 H       4.243149    -1.344485     2.378324      25.47
 H       5.399846     0.114159     2.305061      26.80
 H       6.199361    -1.415643     2.211438      25.22
 C       4.210608    -0.396671    -1.659173      24.99
 O       4.761207    -1.604854    -2.181763     245.73
 H       5.045053    -2.121241    -1.526045      27.31
 C       3.246462     0.219457    -2.532499      58.52
 H       2.868984     0.200341    -3.587406      19.29
 C       2.556356     1.652620    -0.709465      41.86
 C       2.071862     3.013251    -0.104822     115.03
 H       2.460916     3.822734    -0.723175      22.90
 O       2.397273     3.353341     1.409682     256.92
 H       3.228478     3.789842     1.428339      29.71
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 C       0.588453     3.240640    -0.202600      32.57
 H       0.099381     2.734904    -1.079296      18.46
 C      -0.184217     4.519152     0.207944      95.58
 O       0.179135     5.871454    -0.500693     238.80
 H       0.734774     5.668790    -1.202210      32.46
 H       0.081257     4.665509     1.272064      24.46
 H      -1.209264     4.478287    -0.142522      24.02
 C      -1.037845    -1.323378    -0.439073      54.08
 H      -0.620910    -2.308072    -0.566984      19.18
 C      -2.902329     0.208184    -0.969606      33.59
 H      -4.057846     0.509564    -1.366489      24.51
 C      -2.057177     1.349464    -0.407674      -2.92
 O      -2.479068     2.562828    -0.380909     186.63
 C      -3.896445     2.855521    -0.070414     109.71
 H      -4.849076     2.847734    -0.836709      25.13
 H      -4.180592     2.243263     0.775768      27.44
 H      -3.810733     3.974628     0.031185      25.00
 C      -0.663232     1.132157     0.004067      36.73
 O      -0.039878     1.995921     0.848883      92.69
 C      -0.289821    -0.192872    -0.006992      35.63
 H       0.869544    -0.163687     0.191395      18.08
 C      -2.308906    -1.085561    -0.913609      32.96
 C      -3.150228    -2.205441    -1.495859      60.63
 H      -4.278421    -1.821130    -1.694622      23.01
 O      -2.596323    -2.962451    -2.488303     223.56
 H      -3.141461    -3.830455    -2.507695      20.51
 C      -3.460771    -3.474261    -0.235476      65.20
 H      -2.497989    -4.043873    -0.234894      23.22
 O      -3.979197    -2.967194     1.016275     305.36
 H      -3.238985    -2.298271     1.332130      23.28
 C      -4.596462    -4.412977    -0.852931      85.27
 O      -3.979537    -5.307848    -1.856344     217.56
 H      -3.754376    -6.274266    -1.476542      27.63
 H      -5.376101    -3.904334    -1.523297      26.31
 H      -5.153500    -4.845280    -0.015822      27.02
55
name = lig-etoh-frame_118
 C       2.478899     1.292720    -2.084702      35.90
 H       1.544553     1.533644    -2.551684      20.81
 C       3.514522     1.012928     0.275009      62.48
 H       3.832419     1.610871     1.185718      22.80
 C       4.321388    -0.024436    -0.287124      18.31
 O       4.945741    -1.035068     0.466736     219.61
 C       5.211523    -0.905276     1.835646     123.39
 H       4.400236    -1.418290     2.388613      26.35
 H       5.418472     0.166277     2.135860      25.30
 H       6.016144    -1.553867     2.083401      26.96
 C       4.144678    -0.425660    -1.697730      11.78
 O       4.739406    -1.605259    -2.163682     187.59
 H       4.879380    -2.199555    -1.268521      22.33
 C       3.257055     0.244433    -2.472220      51.17
 H       3.210230    -0.123188    -3.535824      25.37
 C       2.587353     1.745304    -0.649491      52.35
 C       2.000739     3.016426    -0.067730     105.74
 H       2.454578     3.898863    -0.750479      20.95
 O       2.365943     3.343409     1.434335     241.82
 H       3.345372     3.663681     1.491002      27.71
 C       0.587706     3.195351    -0.227728      59.63
 H       0.158932     2.831767    -1.123563      21.43
 C      -0.177509     4.500812     0.191333      88.84
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 O       0.212437     5.864091    -0.507493     214.68
 H       0.529996     5.584590    -1.514507      26.54
 H      -0.147223     4.625624     1.325618      24.27
 H      -1.260981     4.435664    -0.065870      22.83
 C      -1.019276    -1.255872    -0.492840      38.22
 H      -0.899379    -2.395610    -0.437674      19.71
 C      -2.915772     0.245712    -0.929667      46.40
 H      -3.768666     0.526232    -1.371703      22.10
 C      -2.040123     1.220245    -0.396817       6.61
 O      -2.526269     2.596203    -0.413923     218.99
 C      -3.871330     2.793753    -0.089596     129.88
 H      -4.531437     2.985713    -0.876376      27.17
 H      -4.153677     2.472934     1.091643      23.37
 H      -3.734012     3.805364     0.300857      25.42
 C      -0.750096     1.117179     0.021798      32.42
 O      -0.021453     2.002737     0.828416     104.62
 C      -0.221684    -0.197670     0.005650      34.16
 H       0.893835    -0.556737     0.275111      18.09
 C      -2.369246    -1.104978    -0.979189      24.27
 C      -3.156210    -2.254188    -1.472755      82.98
 H      -4.130957    -1.752571    -1.521600      25.83
 O      -2.597562    -2.988490    -2.530016     229.95
 H      -3.292696    -3.676690    -2.976947      21.30
 C      -3.463855    -3.419752    -0.219476      85.85
 H      -2.568445    -4.068741    -0.092470      23.44
 O      -3.998823    -3.000881     1.016715     312.78
 H      -3.364115    -2.303034     1.411125      26.62
 C      -4.580089    -4.343094    -0.837260      81.75
 O      -3.998379    -5.335762    -1.932300     226.65
 H      -3.802392    -6.081931    -1.372338      29.59
 H      -5.325881    -3.765746    -1.355850      28.11
 H      -5.299478    -4.981241    -0.087218      26.03
55
name = lig-etoh-frame_119
 C       2.510006     1.396295    -2.019163      68.82
 H       1.497262     1.366990    -2.535562      21.15
 C       3.539123     0.988323     0.149712      74.13
 H       3.841437     1.463523     1.073794      24.22
 C       4.358632    -0.060386    -0.272059      31.80
 O       4.916564    -0.981597     0.455940     242.88
 C       5.259919    -0.939286     1.796175     116.07
 H       4.412540    -1.281318     2.544271      25.03
 H       5.398340     0.100144     2.021740      25.52
 H       6.149093    -1.711322     1.938216      24.26
 C       4.111049    -0.475492    -1.662943       7.79
 O       4.720439    -1.605945    -2.132792     180.61
 H       4.752737    -2.190097    -1.209176      22.71
 C       3.267508     0.253301    -2.492555      50.99
 H       3.429033    -0.385897    -3.376621      21.87
 C       2.677035     1.789592    -0.581746      52.71
 C       1.998543     3.072368    -0.016437     106.59
 H       2.482741     3.898114    -0.565632      22.33
 O       2.332996     3.327214     1.422450     285.79
 H       3.339812     3.517370     1.361408      27.93
 C       0.491840     3.135101    -0.200990      74.08
 H       0.344761     2.974413    -1.367844      20.83
 C      -0.177464     4.518678     0.166281     103.42
 O       0.261990     5.806291    -0.516926     262.90
 H       0.109808     5.616218    -1.514736      29.33
 H      -0.198541     4.686240     1.213188      26.50
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 H      -1.214058     4.253439     0.002885      23.69
 C      -1.036289    -1.224642    -0.549331      34.68
 H      -0.740362    -2.209402    -0.271169      21.38
 C      -2.865424     0.226758    -0.886750      51.34
 H      -3.866903     0.591211    -1.452296      15.33
 C      -2.090723     1.168530    -0.411879      18.39
 O      -2.544917     2.594112    -0.454620     243.41
 C      -3.844316     2.808190    -0.025903     109.12
 H      -4.454154     2.797615    -1.046560      23.19
 H      -4.285763     2.332103     0.873331      26.68
 H      -3.793972     3.860408     0.431469      24.83
 C      -0.782410     1.043664     0.100005       8.91
 O      -0.007788     2.050054     0.764214     172.63
 C      -0.153800    -0.263219    -0.004869      42.67
 H       0.768694    -0.618287     0.419637      18.64
 C      -2.396780    -1.069020    -1.034232      43.62
 C      -3.195355    -2.329912    -1.365031      69.31
 H      -4.262041    -1.847994    -1.686142      25.72
 O      -2.601760    -3.010225    -2.608429     274.24
 H      -3.188623    -3.447754    -3.124345      28.11
 C      -3.479434    -3.387341    -0.246946     103.72
 H      -2.593847    -3.982198     0.008353      23.98
 O      -4.015093    -3.011272     1.024507     339.63
 H      -3.544173    -2.358535     1.506084      31.23
 C      -4.565270    -4.304688    -0.848264      81.78
 O      -4.042560    -5.335362    -1.971326     221.39
 H      -3.679877    -5.971871    -1.320992      28.92
 H      -5.284528    -3.553412    -1.296486      28.06
 H      -5.077934    -5.040190    -0.192493      27.02
55
name = lig-etoh-frame_120
 C       2.522125     1.454063    -1.928789      80.31
 H       1.657121     1.641614    -2.545168      22.25
 C       3.601019     1.011627     0.078570      61.20
 H       3.754589     1.218289     1.174347      22.78
 C       4.309119    -0.075009    -0.343926      35.16
 O       4.921238    -0.995574     0.442535     267.97
 C       5.300768    -0.966952     1.808770     124.78
 H       4.487236    -1.168225     2.476686      26.58
 H       5.654237     0.072263     2.118298      26.16
 H       6.223848    -1.592362     1.809355      26.00
 C       4.104017    -0.493092    -1.579445      26.51
 O       4.702179    -1.629770    -2.088141     251.87
 H       4.822723    -2.194434    -1.430989      30.76
 C       3.294116     0.259087    -2.499338      56.34
 H       3.141000    -0.290657    -3.513818      21.75
 C       2.747456     1.819834    -0.596243      38.96
 C       2.029560     3.127317     0.051389     107.97
 H       2.485637     4.047109    -0.515179      22.67
 O       2.311037     3.304556     1.391503     315.42
 H       3.223088     3.481288     1.351306      30.56
 C       0.417325     3.094953    -0.181367      96.88
 H       0.382418     2.980136    -1.204616      25.30
 C      -0.196315     4.537045     0.135415     102.54
 O       0.290641     5.706367    -0.520733     293.75
 H      -0.017124     5.683199    -1.389201      32.68
 H       0.011737     4.820607     1.262216      24.59
 H      -1.271576     4.273644    -0.090036      23.45
 C      -1.055826    -1.239624    -0.586751      53.05
 H      -0.519487    -2.207439    -0.335233      18.23
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 C      -2.898922     0.166291    -0.918719      46.69
 H      -3.865702     0.496000    -1.292591      19.80
 C      -2.101224     1.263898    -0.388755       2.57
 O      -2.516218     2.540853    -0.485609     238.47
 C      -3.861207     2.875600     0.006730     102.27
 H      -4.542248     2.640266    -0.757858      26.39
 H      -4.404040     1.865899     0.742584      22.76
 H      -3.940743     3.897271     0.252252      26.62
 C      -0.748197     0.947919     0.194408      -5.01
 O      -0.022968     2.104619     0.662696     227.48
 C      -0.169628    -0.302269    -0.040427      47.92
 H       0.822802    -0.537146     0.723802      17.46
 C      -2.360165    -1.072353    -1.052722      40.35
 C      -3.265609    -2.364133    -1.295816      73.52
 H      -4.182542    -2.177048    -1.842311      23.89
 O      -2.590965    -2.998283    -2.654487     174.73
 H      -3.337412    -3.449665    -3.214026      23.48
 C      -3.473703    -3.393981    -0.272124      99.87
 H      -2.488561    -3.893200    -0.075796      24.17
 O      -4.056861    -3.010466     1.031555     284.91
 H      -3.500441    -2.269407     1.574682      24.59
 C      -4.542829    -4.301683    -0.909519      79.64
 O      -4.107361    -5.302006    -1.968043     240.75
 H      -3.373492    -5.885826    -1.438494      26.63
 H      -5.309046    -3.628739    -1.315502      27.96
 H      -4.937830    -4.969780    -0.047304      26.18
55
name = lig-etoh-frame_121
 C       2.559046     1.427353    -1.908174      74.07
 H       1.904007     2.162579    -2.536270      23.65
 C       3.691294     1.072562     0.126191      80.80
 H       3.597277     1.020060     1.231874      23.18
 C       4.241428    -0.073820    -0.354976      25.33
 O       4.950058    -1.051750     0.432440     220.25
 C       5.364531    -0.931697     1.819114     116.32
 H       4.449635    -1.284444     2.530854      25.08
 H       5.891196    -0.050304     2.167343      27.88
 H       6.229182    -1.650126     1.896711      26.73
 C       4.081578    -0.517010    -1.637635      29.11
 O       4.681426    -1.654967    -2.070848     186.19
 H       5.063135    -2.451236    -1.365117      21.26
 C       3.283951     0.292705    -2.467996      51.89
 H       2.833771     0.120474    -3.428097      20.66
 C       2.773585     1.897638    -0.637945      44.86
 C       2.050509     3.163922     0.046671     107.83
 H       2.333066     4.101587    -0.528720      19.32
 O       2.298668     3.280180     1.394470     275.63
 H       3.299016     3.580293     1.535332      27.63
 C       0.446077     3.123502    -0.175487      68.06
 H       0.183493     2.796252    -1.301687      20.83
 C      -0.232488     4.529393     0.147636     115.55
 O       0.321174     5.606594    -0.514452     243.77
 H      -0.012868     5.736932    -1.537604      26.51
 H       0.052674     4.732517     1.121892      26.32
 H      -1.298963     4.572739    -0.046512      25.09
 C      -1.009183    -1.323174    -0.591526      52.55
 H      -0.623499    -2.345112    -0.725334      20.09
 C      -2.929947     0.179045    -0.940385      23.88
 H      -4.045045     0.326679    -1.230821      20.61
 C      -2.069674     1.288286    -0.355984       5.59
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 O      -2.494086     2.516856    -0.499341     203.52
 C      -3.916391     2.863438     0.034828      92.25
 H      -4.765445     2.669914    -0.784337      24.80
 H      -4.018977     2.022605     0.593568      28.80
 H      -4.029616     3.947567     0.261816      25.15
 C      -0.749715     0.944344     0.228832      -2.34
 O      -0.072315     2.109277     0.594661     236.20
 C      -0.203388    -0.307327    -0.024027      70.15
 H       0.617966    -0.487435     0.488540      22.04
 C      -2.336985    -1.153959    -1.045000      19.68
 C      -3.279984    -2.330676    -1.332100      61.36
 H      -4.306575    -2.110075    -1.776173      23.88
 O      -2.587908    -2.976516    -2.670692     174.17
 H      -3.404874    -3.519491    -3.065965      22.62
 C      -3.448128    -3.430802    -0.272061      87.85
 H      -2.470253    -3.898277    -0.194667      25.61
 O      -4.096769    -2.991750     1.033250     301.12
 H      -3.447631    -2.362955     1.372114      28.29
 C      -4.523646    -4.368145    -0.953940      86.95
 O      -4.160034    -5.257429    -1.933943     313.33
 H      -3.327544    -5.626708    -1.759100      33.91
 H      -5.408750    -3.864890    -1.388014      27.88
 H      -4.901867    -4.737421     0.095430      25.89
55
name = lig-etoh-frame_122
 C       2.599571     1.435626    -1.930019      49.99
 H       2.355148     2.274162    -2.542465      24.81
 C       3.731914     1.156779     0.228681      74.72
 H       3.584298     1.139550     1.294019      21.71
 C       4.209615    -0.094935    -0.298385      -0.19
 O       4.985940    -1.102238     0.421792     192.56
 C       5.424428    -0.915678     1.832177     119.02
 H       4.681619    -1.212061     2.483840      28.62
 H       5.915460     0.059777     2.113266      27.31
 H       6.063517    -1.874093     2.030954      26.04
 C       4.050031    -0.548946    -1.749805      17.95
 O       4.666940    -1.718342    -2.086853     202.38
 H       5.158313    -2.166830    -1.304284      22.21
 C       3.221792     0.349313    -2.436221      58.82
 H       2.778069     0.309822    -3.518103      21.17
 C       2.816061     1.973959    -0.621055      42.62
 C       2.044115     3.178517    -0.037173     103.54
 H       2.313100     4.150237    -0.569503      19.18
 O       2.309589     3.264224     1.441148     269.93
 H       3.201158     3.669087     1.611452      29.58
 C       0.494555     3.162234    -0.247061      67.21
 H       0.181491     2.869065    -1.172100      23.62
 C      -0.269883     4.488691     0.164941     101.43
 O       0.367190     5.561112    -0.526908     266.44
 H       0.233737     5.500124    -1.510441      29.44
 H      -0.035496     4.604101     1.328158      24.13
 H      -1.384597     4.643228     0.132050      23.96
 C      -0.958173    -1.436646    -0.604571      27.99
 H      -0.643709    -2.418982    -0.987550      21.01
 C      -2.904283     0.195450    -0.929331      31.29
 H      -4.032390     0.165253    -1.131861      24.11
 C      -2.071841     1.181433    -0.354207       6.64
 O      -2.502065     2.566866    -0.504537     193.64
 C      -3.957261     2.826937    -0.014029      85.44
 H      -4.621390     2.810852    -0.805551      26.56
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 H      -3.950489     2.024852     1.100183      20.68
 H      -3.919246     3.812946     0.473370      25.40
 C      -0.811534     1.024012     0.178780       9.22
 O      -0.127328     2.072653     0.605131     219.72
 C      -0.277337    -0.320445     0.001219      28.50
 H       0.990968    -0.615053     0.264793      18.04
 C      -2.356574    -1.190572    -1.007792      12.23
 C      -3.249600    -2.276193    -1.436923      65.86
 H      -4.291979    -1.756206    -1.476224      24.07
 O      -2.618502    -2.953799    -2.652875     240.36
 H      -3.210904    -3.583230    -2.912092      28.29
 C      -3.457459    -3.457199    -0.299906      74.69
 H      -2.488572    -4.029229    -0.133129      24.71
 O      -4.109316    -2.978403     0.992140     301.23
 H      -3.411047    -2.371289     1.345664      27.36
 C      -4.532318    -4.414884    -0.903873      98.53
 O      -4.197018    -5.240198    -1.928873     286.50
 H      -3.224147    -5.468583    -1.955560      30.72
 H      -5.443578    -3.924003    -1.356340      26.51
 H      -4.994742    -4.915086     0.034870      26.84
55
name = lig-etoh-frame_123
 C       2.655862     1.555777    -1.893832      39.30
 H       2.459687     2.210729    -2.816720      21.25
 C       3.719625     1.204452     0.305589      40.60
 H       3.749185     1.488533     1.428071      17.61
 C       4.197897    -0.126454    -0.265912      -3.84
 O       5.017344    -1.127461     0.416146     183.68
 C       5.490155    -0.937032     1.827318     108.05
 H       4.523956    -0.939214     2.619248      24.96
 H       5.886971     0.077668     1.917888      27.73
 H       6.072209    -1.800179     2.010393      27.31
 C       4.022920    -0.546004    -1.752875      -3.43
 O       4.645036    -1.775121    -2.133165     185.88
 H       5.140415    -1.848248    -1.246994      21.74
 C       3.153851     0.350486    -2.489642      58.24
 H       3.096761     0.160068    -3.519264      24.76
 C       2.885450     1.993955    -0.569664      41.12
 C       2.041114     3.190656    -0.105859      95.93
 H       2.442919     4.202264    -0.526185      20.61
 O       2.312393     3.259304     1.477258     238.54
 H       3.139822     3.728258     1.497516      29.81
 C       0.494276     3.175665    -0.290252      52.33
 H       0.278967     2.970370    -1.448707      18.93
 C      -0.274526     4.448334     0.219929     108.46
 O       0.421145     5.545120    -0.527037     261.48
 H       0.516451     5.175966    -1.494566      29.92
 H      -0.117031     4.536359     1.233307      26.82
 H      -1.354296     4.341987     0.115888      24.51
 C      -0.968688    -1.492554    -0.625286      36.31
 H      -0.388262    -2.409235    -0.982315      20.42
 C      -2.849429     0.110326    -0.896546      56.95
 H      -3.888326     0.306561    -1.080620      25.40
 C      -2.150798     1.134602    -0.387042       7.31
 O      -2.539050     2.609939    -0.496730     232.52
 C      -3.912058     2.742175     0.007046     126.15
 H      -4.661272     2.766075    -0.883927      25.87
 H      -4.274118     2.419812     0.890262      27.77
 H      -3.778250     3.716822     0.490716      25.74
 C      -0.858070     1.034433     0.078653      15.43
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 O      -0.149583     2.054520     0.660942     172.15
 C      -0.280963    -0.379630     0.016659      15.61
 H       0.668146    -0.432621     0.011071      21.96
 C      -2.343098    -1.162160    -0.947185      34.93
 C      -3.215397    -2.247367    -1.503900      73.39
 H      -4.176189    -1.690443    -1.540653      24.21
 O      -2.662285    -2.907141    -2.619023     210.11
 H      -3.158536    -3.841372    -2.847283      20.33
 C      -3.503280    -3.464730    -0.343145      90.31
 H      -2.638879    -4.032160    -0.044095      24.30
 O      -4.090324    -2.966235     0.910487     321.24
 H      -3.448280    -2.345489     1.490244      24.70
 C      -4.591453    -4.421751    -0.781545      95.63
 O      -4.202141    -5.265748    -1.972827     235.90
 H      -3.154746    -5.364728    -1.987229      27.95
 H      -5.384695    -3.760620    -1.131432      26.33
 H      -4.991543    -5.307859    -0.135657      24.69
55
name = lig-etoh-frame_124
 C       2.742974     1.676422    -1.911269      52.12
 H       2.242253     2.197077    -2.724857      21.68
 C       3.699754     1.181612     0.349937      39.38
 H       3.985579     1.663086     1.242406      20.21
 C       4.191817    -0.132777    -0.248841      -6.24
 O       5.036212    -1.131784     0.414849     194.45
 C       5.477349    -0.931990     1.812197     112.03
 H       4.699658    -0.753036     2.412610      28.03
 H       6.063026     0.017981     1.762662      26.81
 H       6.333931    -1.765195     2.054136      24.69
 C       3.971583    -0.506369    -1.672900     -10.28
 O       4.603803    -1.795144    -2.169361     119.95
 H       5.292324    -1.758624    -1.266617      19.62
 C       3.138191     0.315341    -2.517801      48.92
 H       3.335949     0.033023    -3.647817      23.90
 C       2.938760     1.991313    -0.529599      39.46
 C       2.063821     3.206558    -0.091980     100.48
 H       2.491318     4.128044    -0.479218      23.57
 O       2.303190     3.267492     1.475831     224.21
 H       3.191487     3.838223     1.393008      26.37
 C       0.462204     3.152806    -0.309750      68.35
 H       0.338873     3.009588    -1.338150      20.67
 C      -0.231536     4.400243     0.231731      99.58
 O       0.449308     5.532053    -0.522090     232.52
 H       0.863464     4.987835    -1.332525      30.15
 H      -0.025153     4.583373     1.360555      23.81
 H      -1.259682     4.115709    -0.115533      22.21
 C      -0.977944    -1.466330    -0.621698      59.81
 H      -0.360694    -2.293722    -0.776297      21.78
 C      -2.845979     0.015198    -0.856313      40.67
 H      -3.910440     0.432286    -1.211034      20.95
 C      -2.193405     1.216954    -0.415544      -3.55
 O      -2.593540     2.574095    -0.474985     255.39
 C      -3.862520     2.748630    -0.003251     119.75
 H      -4.645399     2.658617    -0.738154      26.77
 H      -4.571164     2.066530     0.977050      22.06
 H      -3.847084     3.859733     0.194566      25.09
 C      -0.859646     0.948612    -0.010549      16.43
 O      -0.146908     2.048863     0.695018     133.93
 C      -0.329575    -0.410741    -0.016068      28.28
 H       0.984367    -0.259752    -0.024188      17.52
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 C      -2.287963    -1.206825    -0.910731      47.37
 C      -3.211851    -2.264412    -1.485731      67.54
 H      -4.235177    -1.850627    -1.944197      21.80
 O      -2.699738    -2.872062    -2.622600     254.85
 H      -3.104501    -3.793364    -2.636151      22.36
 C      -3.551188    -3.443902    -0.352757      94.92
 H      -2.576772    -3.987458    -0.105968      22.12
 O      -4.068090    -2.935773     0.834229     362.29
 H      -3.509805    -2.455274     1.387726      29.57
 C      -4.662170    -4.464050    -0.701387      85.72
 O      -4.187723    -5.278546    -2.030781     275.32
 H      -3.295312    -5.405783    -1.833583      32.41
 H      -5.503156    -3.709243    -0.898926      25.89
 H      -4.884183    -5.275146    -0.051544      26.48
55
name = lig-etoh-frame_125
 C       2.841257     1.696815    -1.979156      35.36
 H       2.018143     2.381586    -2.416199      17.61
 C       3.701261     1.092423     0.330521      53.42
 H       4.240427     1.611370     1.210605      22.10
 C       4.190981    -0.112810    -0.219155       2.91
 O       5.037551    -1.125170     0.407723     196.49
 C       5.521047    -0.897531     1.743912     116.98
 H       4.572930    -0.704522     2.543441      23.85
 H       6.231926    -0.052916     1.742625      27.21
 H       6.129946    -1.633335     2.072160      28.44
 C       3.906832    -0.482190    -1.581162       3.95
 O       4.560121    -1.748663    -2.153606     193.11
 H       5.258710    -2.065722    -1.695810      27.69
 C       3.188945     0.315635    -2.496999      58.75
 H       3.224489     0.137346    -3.514270      28.27
 C       2.944822     1.990651    -0.545650      36.07
 C       2.093497     3.183884     0.006090     100.23
 H       2.503490     4.178601    -0.545732      22.24
 O       2.304688     3.304998     1.431186     303.47
 H       3.114634     3.818743     1.547686      28.95
 C       0.475154     3.091080    -0.238673      71.64
 H       0.158632     2.843030    -1.336476      19.12
 C      -0.155035     4.361536     0.202810     112.26
 O       0.466403     5.503846    -0.503051     299.98
 H       0.927999     5.219267    -1.235917      35.12
 H      -0.059623     4.543565     1.252200      26.25
 H      -1.182681     4.317114    -0.156369      25.25
 C      -0.947567    -1.423486    -0.587434      57.65
 H      -0.450585    -2.487574    -0.610465      21.31
 C      -2.908909     0.057003    -0.816076      47.58
 H      -3.828112     0.055385    -1.301815      19.51
 C      -2.165877     1.259600    -0.444716      -0.61
 O      -2.624901     2.480926    -0.452932     255.46
 C      -3.929947     2.800224     0.032940     112.16
 H      -4.648028     2.514730    -0.852477      24.68
 H      -4.052270     2.029368     0.617463      30.81
 H      -4.088220     3.856119     0.081006      25.40
 C      -0.848494     0.886442    -0.048882      15.66
 O      -0.132549     2.027071     0.671007     196.83
 C      -0.282001    -0.343618    -0.075519      34.32
 H       0.636803    -0.403965     0.161301      22.25
 C      -2.294412    -1.311929    -0.919016      37.54
 C      -3.271196    -2.314592    -1.440231      81.29
 H      -4.168917    -1.920661    -1.881977      24.95
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 O      -2.699935    -2.866498    -2.658690     290.73
 H      -3.123343    -3.735155    -2.628690      22.84
 C      -3.561062    -3.428198    -0.360278      88.91
 H      -2.573576    -3.892393    -0.319439      22.99
 O      -4.075542    -2.889933     0.785673     328.86
 H      -3.330969    -2.421966     1.316823      23.69
 C      -4.707511    -4.498369    -0.705224      72.55
 O      -4.193691    -5.257787    -2.060810     233.81
 H      -3.339177    -5.639894    -1.593856      27.32
 H      -5.688764    -4.069760    -0.819385      27.48
 H      -4.735152    -5.187351     0.327236      25.20
55
name = lig-etoh-frame_126
 C       2.897584     1.670015    -2.003602      32.18
 H       2.107444     2.345657    -2.298819      17.64
 C       3.723125     1.038300     0.292441      71.19
 H       4.208602     1.304285     1.191215      25.00
 C       4.206051    -0.122973    -0.194060      17.56
 O       5.025455    -1.104963     0.394874     229.11
 C       5.533811    -0.816192     1.694003     120.95
 H       4.829538    -0.720797     2.389405      28.14
 H       6.238047     0.028872     1.789760      27.45
 H       5.946252    -1.924802     2.100235      24.15
 C       3.885060    -0.515914    -1.519752      17.19
 O       4.473382    -1.654428    -2.138063     178.01
 H       5.279641    -2.342751    -1.879611      22.46
 C       3.261853     0.392416    -2.423827      73.05
 H       3.015717     0.146376    -3.536083      24.93
 C       2.944305     1.958722    -0.596053      61.27
 C       2.133074     3.145593     0.079923     116.30
 H       2.373330     4.015172    -0.468678      23.22
 O       2.304554     3.353775     1.397482     329.57
 H       3.117486     3.799165     1.645081      29.98
 C       0.517727     2.980751    -0.152217      80.44
 H       0.156076     2.712312    -1.139073      20.85
 C      -0.091997     4.361777     0.132776     109.74
 O       0.480615     5.495604    -0.454904     273.49
 H       0.873866     5.358196    -1.424412      28.23
 H      -0.080950     4.482009     1.262986      24.93
 H      -1.188679     4.542698    -0.038929      24.25
 C      -0.933499    -1.460446    -0.555664      38.03
 H      -0.585244    -2.422039    -0.472673      19.24
 C      -2.942004     0.084259    -0.792075      44.88
 H      -3.961854    -0.161235    -1.326834      16.71
 C      -2.145550     1.167894    -0.482454      13.47
 O      -2.623456     2.445145    -0.442075     227.29
 C      -4.031434     2.815734    -0.017049      70.12
 H      -4.592898     2.445174    -0.843646      26.04
 H      -3.942578     1.942387     0.990102      22.09
 H      -4.213789     3.882372     0.298553      25.01
 C      -0.828115     0.955139    -0.036880      10.39
 O      -0.114595     1.981340     0.617527     244.15
 C      -0.221390    -0.274225    -0.143338      35.74
 H       0.863911    -0.580613     0.523012      16.10
 C      -2.347536    -1.318500    -0.920961      19.62
 C      -3.324309    -2.384195    -1.414795      57.51
 H      -4.354190    -1.717726    -1.532175      24.71
 O      -2.688022    -2.885453    -2.697117     198.49
 H      -3.170141    -3.857576    -2.901436      19.37
 C      -3.588818    -3.434177    -0.421545      84.92
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 H      -2.600041    -3.993622    -0.340113      21.93
 O      -4.081095    -2.819974     0.789676     305.25
 H      -3.268526    -2.357860     1.237094      25.09
 C      -4.690233    -4.545840    -0.719632      91.80
 O      -4.197064    -5.220469    -2.026954     264.09
 H      -3.671486    -6.007012    -1.577524      28.18
 H      -5.819676    -4.433287    -0.916653      26.99
 H      -4.604610    -5.066713     0.157056      29.00
55
name = lig-etoh-frame_127
 C       2.901368     1.661998    -1.940403      62.00
 H       2.280027     2.238307    -2.717464      22.33
 C       3.729606     1.049903     0.252008      60.10
 H       3.948051     1.215204     1.371325      21.12
 C       4.228311    -0.190462    -0.218933      36.75
 O       5.016895    -1.074746     0.388669     242.13
 C       5.569791    -0.796334     1.669807     122.48
 H       4.645229    -0.528328     2.490929      24.00
 H       6.288099     0.045986     1.748075      27.98
 H       5.867922    -1.711041     1.891313      28.41
 C       3.904396    -0.556134    -1.507192      36.88
 O       4.372941    -1.573484    -2.153303     213.75
 H       5.030068    -2.232886    -1.670413      24.74
 C       3.336222     0.452922    -2.381999      82.31
 H       2.952117     0.065720    -3.297377      21.99
 C       2.978822     1.901979    -0.591510      36.94
 C       2.150707     3.059390     0.064515     108.86
 H       2.285409     4.084704    -0.595094      21.42
 O       2.307471     3.402353     1.432688     268.77
 H       3.295085     3.795604     1.554213      26.96
 C       0.571128     2.895890    -0.108057      76.23
 H       0.465710     2.661529    -1.222289      20.35
 C      -0.083206     4.372572     0.107089     111.11
 O       0.537946     5.520472    -0.423680     262.25
 H       0.449162     5.342997    -1.446658      29.23
 H       0.061712     4.463433     1.212120      25.63
 H      -1.177697     4.378050    -0.038344      25.03
 C      -0.986710    -1.468368    -0.533437      37.32
 H      -0.483688    -2.524076    -0.356584      15.91
 C      -2.967547    -0.012837    -0.820978      56.05
 H      -3.978047     0.255790    -1.072675      19.31
 C      -2.167243     1.084845    -0.504311       4.07
 O      -2.610988     2.468085    -0.440236     213.58
 C      -4.081451     2.713632    -0.018061     117.85
 H      -4.832267     2.418896    -0.808248      25.68
 H      -4.395700     2.479198     0.928798      28.29
 H      -4.111476     3.732843     0.351322      27.02
 C      -0.781225     1.041901    -0.020742       1.69
 O      -0.100660     1.926004     0.601395     252.83
 C      -0.128678    -0.290799    -0.175268      31.75
 H       0.636752    -0.408743     0.470562      19.08
 C      -2.371236    -1.247456    -0.895048      32.52
 C      -3.360336    -2.395327    -1.437102      76.50
 H      -4.301207    -1.882107    -1.419315      27.13
 O      -2.707967    -2.925285    -2.726345     263.65
 H      -3.079673    -3.686978    -3.042611      27.73
 C      -3.645253    -3.478042    -0.463110      92.09
 H      -2.808413    -4.114603    -0.196950      21.93
 O      -4.071630    -2.749475     0.805908     346.22
 H      -3.396310    -2.280974     1.221877      31.55
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 C      -4.650141    -4.579012    -0.783918     106.21
 O      -4.200445    -5.213149    -1.951397     309.60
 H      -4.008823    -6.100825    -1.824422      33.19
 H      -5.693658    -4.444434    -0.964098      27.80
 H      -4.463665    -5.403081     0.138527      25.37
55
name = lig-etoh-frame_128
 C       2.860298     1.675549    -1.907793      88.98
 H       2.657532     2.129862    -2.884550      24.87
 C       3.747164     1.049310     0.253179      63.96
 H       3.501510     1.282119     1.289346      20.30
 C       4.223915    -0.208715    -0.256584      36.88
 O       5.035202    -1.068420     0.400597     243.41
 C       5.546227    -0.754420     1.687272     116.63
 H       4.825410    -0.427362     2.282159      28.46
 H       6.346390    -0.001404     1.601821      27.48
 H       6.158749    -1.803091     1.985299      24.20
 C       3.908708    -0.499402    -1.534111      37.23
 O       4.297311    -1.577972    -2.201458     253.40
 H       4.703234    -1.997769    -1.480077      28.07
 C       3.400064     0.448745    -2.341919      59.81
 H       3.050327     0.025677    -3.316640      19.71
 C       3.008606     1.891088    -0.509527      58.44
 C       2.137706     2.998518     0.007701     114.34
 H       2.291529     3.832227    -0.575074      27.90
 O       2.350560     3.450391     1.492630     293.37
 H       3.249662     3.711631     1.400459      32.19
 C       0.649692     2.889919    -0.161806      67.37
 H       0.766726     2.626077    -1.240678      22.15
 C      -0.086678     4.343732     0.150652     100.81
 O       0.594579     5.545645    -0.433732     257.42
 H       0.238368     5.457743    -1.292277      32.56
 H       0.124733     4.496396     1.191495      26.59
 H      -1.127283     4.127221    -0.172636      23.82
 C      -1.018290    -1.435635    -0.500014      53.91
 H      -0.594216    -2.380872    -0.400186      17.07
 C      -2.988469    -0.050141    -0.855751      55.15
 H      -3.986450     0.468666    -0.848986      17.62
 C      -2.157249     1.086638    -0.479783       2.90
 O      -2.641556     2.473527    -0.428139     185.55
 C      -4.098519     2.630173    -0.023965     108.86
 H      -4.960598     2.496458    -0.730250      25.97
 H      -4.745838     2.365419     1.062116      23.74
 H      -3.968272     3.775666    -0.050740      25.21
 C      -0.778565     0.961275    -0.080770      14.98
 O      -0.067713     1.913189     0.650969     224.42
 C      -0.156158    -0.318457    -0.205211      38.31
 H       0.925490    -0.368829     0.494445      15.50
 C      -2.379848    -1.260675    -0.885561      33.13
 C      -3.332693    -2.394519    -1.477479      57.73
 H      -4.466956    -1.973690    -1.767592      24.34
 O      -2.733435    -2.928924    -2.738079     223.24
 H      -3.225375    -3.773759    -3.063132      24.79
 C      -3.684992    -3.519739    -0.419563      86.50
 H      -2.796994    -4.123519    -0.090192      22.66
 O      -4.088955    -2.707177     0.799443     316.39
 H      -3.322149    -2.159646     1.263878      24.47
 C      -4.614292    -4.654058    -0.787734     110.10
 O      -4.186494    -5.222067    -1.926332     261.46
 H      -4.301444    -6.253388    -2.001711      29.12
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 H      -5.695607    -4.172483    -0.850824      27.74
 H      -4.583602    -5.367722    -0.100158      29.42
55
name = lig-etoh-frame_129
 C       2.862372     1.651457    -1.915527      84.82
 H       2.699235     2.450088    -2.688005      29.26
 C       3.749528     1.017044     0.302538      62.26
 H       3.399480     1.223593     1.324848      18.44
 C       4.217948    -0.158604    -0.237063      31.38
 O       5.063583    -1.099774     0.411556     226.13
 C       5.581708    -0.751662     1.691463     119.38
 H       4.722199    -0.313916     2.466157      25.25
 H       6.299513     0.062691     1.486832      27.41
 H       6.118487    -1.480834     2.167237      28.64
 C       3.921764    -0.426701    -1.584316      27.80
 O       4.250047    -1.648197    -2.253865     151.81
 H       4.544555    -2.208698    -1.325347      21.54
 C       3.383029     0.478925    -2.356382      24.14
 H       3.365882     0.193704    -3.447865      17.39
 C       2.999170     1.924419    -0.471721     101.46
 C       2.127921     2.972207     0.037153     102.70
 H       2.485243     3.917228    -0.697834      21.74
 O       2.404764     3.478373     1.517255     228.28
 H       3.378224     3.776956     1.445208      29.69
 C       0.715147     2.925751    -0.238563      68.56
 H       0.559004     2.579229    -1.288888      20.82
 C      -0.044832     4.280867     0.188298      89.29
 O       0.629358     5.544855    -0.443592     157.47
 H       0.146229     5.724840    -1.403256      28.12
 H      -0.028335     4.468294     1.340519      25.05
 H      -1.051507     4.124260    -0.245476      23.01
 C      -1.033386    -1.388381    -0.479668      61.00
 H      -0.658257    -2.475276    -0.489613      19.16
 C      -2.979963     0.053520    -0.856081      51.69
 H      -4.134888     0.110040    -0.855711      27.64
 C      -2.133070     1.120834    -0.439719       3.34
 O      -2.705118     2.418435    -0.399448     216.21
 C      -4.131218     2.634209    -0.013649     122.74
 H      -4.797566     2.335779    -0.877103      27.28
 H      -4.370259     2.108093     0.842178      28.88
 H      -4.097342     3.660979    -0.327005      25.79
 C      -0.791473     0.845666    -0.149792      15.38
 O      -0.028350     1.914122     0.694728     139.50
 C      -0.210300    -0.354783    -0.179460      35.54
 H       0.843579    -0.452880    -0.029831      18.15
 C      -2.412555    -1.342681    -0.910069      38.63
 C      -3.321915    -2.423553    -1.527099      71.29
 H      -4.191857    -2.000946    -1.969082      24.45
 O      -2.753525    -2.927414    -2.749725     231.00
 H      -3.377653    -3.787623    -2.850659      23.83
 C      -3.646502    -3.520874    -0.317882      89.57
 H      -2.662593    -3.932217    -0.106417      24.80
 O      -4.128867    -2.687875     0.778261     353.68
 H      -3.305197    -2.270781     1.183970      24.21
 C      -4.655464    -4.669319    -0.737507      90.45
 O      -4.148969    -5.263082    -1.986376     254.94
 H      -4.624880    -6.163010    -2.006887      28.98
 H      -5.544863    -4.087605    -0.777351      27.61
 H      -4.813278    -5.511538     0.189812      24.79
55
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name = lig-etoh-frame_130
 C       2.888115     1.695440    -1.894525      44.91
 H       2.528647     2.667938    -2.265495      18.22
 C       3.692972     1.021122     0.383659      50.76
 H       3.706671     1.022459     1.532494      19.88
 C       4.245095    -0.135280    -0.210600      16.23
 O       5.074491    -1.150255     0.416023     220.68
 C       5.593260    -0.685167     1.711488     116.15
 H       4.850445    -0.434649     2.387701      28.58
 H       6.152805     0.252668     1.546881      28.32
 H       6.141979    -1.557438     2.350318      25.47
 C       3.984692    -0.450199    -1.609658      20.63
 O       4.218530    -1.725292    -2.245059     207.89
 H       4.432201    -2.501540    -1.741945      25.31
 C       3.328652     0.545260    -2.482799      76.23
 H       3.572508     0.459904    -3.518465      26.07
 C       2.986906     1.910362    -0.495258      34.00
 C       2.194036     3.053655     0.097455     118.50
 H       2.484365     3.838546    -0.473993      23.53
 O       2.463772     3.483340     1.497157     270.97
 H       3.418754     3.889363     1.571954      28.00
 C       0.700530     2.965140    -0.268780      72.28
 H       0.235765     2.679651    -1.260824      19.25
 C       0.019867     4.234762     0.181307     104.93
 O       0.638742     5.526037    -0.445088     222.72
 H       0.229023     5.786558    -1.279572      31.01
 H      -0.145364     4.320867     1.198986      27.93
 H      -1.003677     4.265502    -0.184659      24.86
 C      -1.097360    -1.465770    -0.508626      50.98
 H      -0.601512    -2.443827    -0.590806      20.78
 C      -2.960940     0.087029    -0.839543      59.54
 H      -4.000224    -0.092627    -0.999686      25.41
 C      -2.176263     1.152065    -0.410220       8.48
 O      -2.745022     2.354387    -0.358690     239.03
 C      -4.136768     2.633121    -0.096204      93.79
 H      -4.561688     1.943173    -0.888682      24.67
 H      -4.166424     2.002665     0.983345      23.48
 H      -4.417967     3.774168    -0.073553      23.86
 C      -0.784629     0.871066    -0.143778      33.70
 O       0.003441     1.895405     0.684595     151.55
 C      -0.253949    -0.413437    -0.165389      31.26
 H       0.940004    -0.595760    -0.292756      18.43
 C      -2.449948    -1.327233    -0.934902      28.04
 C      -3.298475    -2.465418    -1.537690      53.41
 H      -4.274897    -1.763768    -1.891827      23.21
 O      -2.767743    -2.960106    -2.763303     275.90
 H      -3.223398    -3.733435    -2.841980      28.59
 C      -3.580835    -3.498316    -0.245232      84.49
 H      -2.529253    -3.833885    -0.051466      24.69
 O      -4.173637    -2.694040     0.749901     356.75
 H      -3.439700    -2.360146     1.220742      28.56
 C      -4.677573    -4.663218    -0.629000      83.18
 O      -4.136285    -5.309424    -2.036687     272.45
 H      -4.746286    -5.985376    -2.107331      33.34
 H      -5.677908    -4.126163    -0.919774      26.46
 H      -4.870230    -5.320633     0.079124      27.90
55
name = lig-etoh-frame_131
 C       2.912454     1.797175    -1.833697      52.73
 H       2.342464     2.620393    -2.268468      21.03
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 C       3.632519     1.008760     0.457181      53.32
 H       3.952574     1.070602     1.453570      22.34
 C       4.285706    -0.163708    -0.228030      -5.15
 O       5.073276    -1.184026     0.436092     189.02
 C       5.610862    -0.635098     1.731277     105.47
 H       4.624085    -0.483530     2.457674      24.02
 H       6.104645     0.345371     1.679306      27.56
 H       6.180355    -1.467212     2.119325      26.84
 C       4.032057    -0.491308    -1.638882      -4.39
 O       4.190229    -1.771165    -2.239303     205.46
 H       4.428827    -2.630683    -1.866087      24.96
 C       3.326899     0.571329    -2.593806      50.69
 H       3.574901     0.676485    -3.734475      25.53
 C       2.983205     1.859742    -0.458334      28.26
 C       2.281642     3.147416     0.141552      98.12
 H       2.563444     4.187046    -0.487973      22.61
 O       2.516401     3.471805     1.471567     305.19
 H       3.333127     3.923176     1.485516      29.07
 C       0.639187     2.983539    -0.228968      75.08
 H       0.394152     2.812781    -1.257122      20.12
 C       0.044645     4.253892     0.116683      99.99
 O       0.654140     5.491258    -0.406343     238.29
 H       0.212635     5.603540    -1.236470      31.78
 H      -0.005789     4.274679     1.315233      24.68
 H      -1.039771     4.317885    -0.190690      24.22
 C      -1.166393    -1.592046    -0.569926      41.77
 H      -0.591110    -2.521507    -0.690456      19.52
 C      -2.934420    -0.003357    -0.829449      47.29
 H      -4.075534     0.161920    -1.224069      19.16
 C      -2.231650     1.137812    -0.385676      10.56
 O      -2.737438     2.370748    -0.316400     264.11
 C      -4.133533     2.552862    -0.155622     143.31
 H      -4.709479     1.884283    -0.750022      27.76
 H      -4.371549     2.304291     0.874739      27.34
 H      -4.547002     3.486400     0.136336      26.27
 C      -0.761849     0.970401    -0.062653      31.78
 O       0.026140     1.864427     0.621174     206.80
 C      -0.285509    -0.465629    -0.174810      22.09
 H       0.846719    -0.682441    -0.322126      19.35
 C      -2.451902    -1.249716    -0.951579      31.98
 C      -3.310219    -2.448386    -1.510591      66.32
 H      -4.295081    -1.970214    -1.583981      25.35
 O      -2.765046    -2.996348    -2.771218     218.60
 H      -3.117349    -4.010383    -2.989441      19.40
 C      -3.541301    -3.481318    -0.253254      89.27
 H      -2.606661    -3.913540     0.126371      24.22
 O      -4.218991    -2.710965     0.730594     313.10
 H      -3.611832    -2.291396     1.518141      23.94
 C      -4.654751    -4.589795    -0.597411      77.25
 O      -4.139684    -5.334791    -2.033357     205.70
 H      -4.926471    -5.969775    -2.339247      31.15
 H      -5.586062    -4.259521    -1.004038      25.99
 H      -4.833245    -5.505959     0.241930      24.00
55
name = lig-etoh-frame_132
 C       2.946492     1.823114    -1.824811      46.93
 H       2.314460     2.447916    -2.488534      20.10
 C       3.627210     0.918377     0.447333      63.54
 H       4.007184     1.408884     1.469344      21.06
 C       4.299820    -0.207980    -0.270457       2.40
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 O       5.070384    -1.176397     0.468893     203.86
 C       5.563804    -0.606326     1.745654     110.42
 H       4.731231    -0.631719     2.398051      25.84
 H       6.101663     0.360019     1.680078      27.24
 H       6.363069    -1.410017     2.015707      25.50
 C       4.034214    -0.501230    -1.694573      -3.58
 O       4.164842    -1.782109    -2.250382     138.72
 H       4.591608    -2.578064    -1.579041      20.57
 C       3.382527     0.614303    -2.607266      52.53
 H       3.347949     0.647151    -3.654783      24.25
 C       2.969675     1.868638    -0.350434      50.10
 C       2.337660     3.238518     0.099454     102.71
 H       2.547601     4.047571    -0.426351      28.63
 O       2.559240     3.450181     1.473624     300.74
 H       3.436892     4.045110     1.420558      25.92
 C       0.634481     2.973628    -0.173801      63.42
 H       0.795599     2.750211    -1.298550      18.20
 C      -0.008908     4.332426     0.121044     119.76
 O       0.672700     5.450530    -0.357296     233.84
 H       0.260869     5.394550    -1.369853      27.63
 H       0.200544     4.383368     1.124551      27.03
 H      -1.039579     4.275946    -0.177466      25.25
 C      -1.153294    -1.636535    -0.614957      30.82
 H      -0.769619    -2.717082    -0.823114      16.67
 C      -2.977588    -0.025307    -0.838538      56.55
 H      -3.807922     0.332508    -1.253512      19.67
 C      -2.207472     1.080084    -0.346433      16.88
 O      -2.721801     2.440664    -0.280206     223.58
 C      -4.160589     2.446491    -0.158983     113.92
 H      -5.010438     1.971420    -0.794780      25.56
 H      -4.582099     2.132568     1.007180      24.05
 H      -4.449393     3.576519    -0.194128      25.41
 C      -0.786345     0.966443     0.015980      10.10
 O       0.059908     1.861289     0.539695     241.74
 C      -0.358658    -0.491458    -0.210654      24.17
 H       0.798856    -0.680571    -0.125712      17.98
 C      -2.443528    -1.283324    -0.993064      35.68
 C      -3.317841    -2.433082    -1.455978      66.70
 H      -4.534753    -2.308265    -1.497188      23.58
 O      -2.766696    -3.034181    -2.770016     221.94
 H      -3.018414    -4.004442    -2.842241      21.93
 C      -3.530868    -3.474468    -0.293002      97.40
 H      -2.730775    -4.044991     0.221679      23.69
 O      -4.267252    -2.714291     0.743874     322.29
 H      -3.835562    -2.379908     1.539313      27.69
 C      -4.587653    -4.571483    -0.618180      90.76
 O      -4.157134    -5.352532    -1.991534     273.25
 H      -4.950803    -5.755866    -2.461784      33.32
 H      -5.591831    -4.139945    -0.901493      27.59
 H      -4.603999    -5.282056     0.098492      29.03
55
name = lig-etoh-frame_133
 C       2.985831     1.751532    -1.840142      67.54
 H       2.462149     2.400030    -2.537550      24.38
 C       3.670341     0.842723     0.398566      63.20
 H       3.864808     1.350173     1.258248      22.84
 C       4.279919    -0.242523    -0.312870      12.93
 O       5.062349    -1.141318     0.488065     206.39
 C       5.536491    -0.631742     1.734172     109.04
 H       4.734002    -0.682144     2.612125      23.99
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 H       5.937648     0.386263     1.549127      26.71
 H       6.469144    -1.237736     2.031037      25.71
 C       4.000331    -0.463743    -1.755782      11.29
 O       4.161611    -1.794499    -2.245230     205.85
 H       4.620007    -2.068661    -1.509791      25.92
 C       3.472514     0.654332    -2.486781      44.69
 H       3.084332     0.441867    -3.589542      19.21
 C       2.957854     1.925507    -0.320356      35.42
 C       2.321129     3.214396     0.082424      82.05
 H       2.634639     4.156545    -0.685888      23.86
 O       2.622706     3.455621     1.494918     309.25
 H       3.428472     4.024863     1.580832      28.80
 C       0.713369     2.980854    -0.177879      71.40
 H       0.834412     2.653732    -1.159055      20.84
 C      -0.076955     4.366004     0.173449     104.38
 O       0.679825     5.426894    -0.368459     254.50
 H       0.702584     5.430671    -1.317271      33.17
 H       0.118639     4.512606     1.329719      24.57
 H      -1.192846     4.314842    -0.076690      23.79
 C      -1.105531    -1.616657    -0.657694      39.28
 H      -0.876521    -2.616782    -0.809711      17.90
 C      -2.984882     0.018534    -0.833245      43.31
 H      -4.017068     0.392297    -1.434260      15.77
 C      -2.140017     1.054878    -0.294457       9.89
 O      -2.723510     2.466309    -0.255123     172.52
 C      -4.249752     2.410051    -0.108502     115.16
 H      -4.767036     1.981086    -0.962308      26.27
 H      -4.514376     1.930002     0.811656      27.82
 H      -4.241131     3.401794    -0.526178      25.63
 C      -0.860004     0.831013     0.040550       5.90
 O       0.107019     1.874543     0.482105     212.38
 C      -0.405471    -0.495532    -0.247194      44.04
 H       0.663791    -0.610194     0.300007      17.31
 C      -2.468521    -1.372386    -1.046599      12.16
 C      -3.355444    -2.476213    -1.420238      87.27
 H      -4.363182    -2.247354    -1.704819      25.55
 O      -2.771326    -3.051837    -2.738717     246.83
 H      -3.055376    -3.981429    -2.614535      22.44
 C      -3.537351    -3.482787    -0.300496     100.94
 H      -2.674838    -4.002353     0.136885      23.17
 O      -4.334291    -2.723771     0.752209     292.54
 H      -3.726875    -2.490404     1.494358      26.25
 C      -4.516644    -4.561310    -0.730036      90.76
 O      -4.174945    -5.347816    -1.923869     347.13
 H      -4.959419    -5.480765    -2.385025      35.33
 H      -5.504769    -4.013611    -0.618434      28.22
 H      -4.453482    -5.326339     0.221132      26.27
55
name = lig-etoh-frame_134
 C       3.001062     1.711263    -1.791237      95.30
 H       2.632292     2.511023    -2.450044      28.21
 C       3.685457     0.851204     0.287311      39.27
 H       3.883391     0.984289     1.490346      20.40
 C       4.239081    -0.249593    -0.338392      16.28
 O       5.043053    -1.122012     0.475719     224.97
 C       5.521401    -0.649398     1.725622     119.48
 H       4.904677    -0.696452     2.648512      26.91
 H       5.675526     0.424767     1.537046      27.50
 H       6.419863    -1.196784     2.034683      27.16
 C       3.974871    -0.431363    -1.758555      31.59
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 O       4.166326    -1.769133    -2.235734     184.32
 H       4.802562    -2.010429    -1.444850      22.61
 C       3.550323     0.615997    -2.394619      62.62
 H       3.081029     0.339639    -3.263655      20.41
 C       2.994415     1.923689    -0.423090      29.49
 C       2.287926     3.171534     0.096440     103.95
 H       2.561995     3.882976    -0.528525      25.13
 O       2.671672     3.471526     1.518380     315.68
 H       3.506631     3.978746     1.605202      28.27
 C       0.782584     3.019279    -0.194892      50.89
 H       0.603041     2.776805    -1.332012      17.14
 C      -0.114818     4.344436     0.247375     102.80
 O       0.693118     5.441844    -0.389669     235.29
 H       0.984806     5.330876    -1.321662      31.73
 H      -0.185421     4.496613     1.287187      26.61
 H      -1.150590     4.386611    -0.000129      25.61
 C      -1.120217    -1.562645    -0.719699      46.00
 H      -0.593990    -2.660130    -0.678003      18.42
 C      -2.978214     0.030199    -0.862281      53.42
 H      -3.861472     0.163675    -1.249646      20.50
 C      -2.179866     1.092070    -0.275079       5.31
 O      -2.723972     2.418801    -0.225478     198.62
 C      -4.281710     2.405717    -0.129925      86.21
 H      -4.434465     1.765257    -1.069138      23.70
 H      -4.609024     1.902086     0.913803      25.27
 H      -4.467534     3.538046    -0.361403      24.45
 C      -0.858670     0.718885     0.035245      15.69
 O       0.134773     1.842643     0.470534     184.09
 C      -0.374703    -0.498867    -0.214390      53.70
 H       0.530008    -0.627886     0.359940      17.40
 C      -2.499557    -1.359979    -1.062599       8.35
 C      -3.375846    -2.528728    -1.440324      71.14
 H      -4.295996    -1.884176    -1.933472      21.85
 O      -2.778570    -3.069551    -2.680999     225.76
 H      -3.084651    -4.126646    -2.562078      17.73
 C      -3.562312    -3.487395    -0.291220     100.18
 H      -2.525277    -3.773032     0.016680      23.38
 O      -4.383092    -2.752413     0.755062     296.78
 H      -3.553745    -2.549548     1.388683      22.56
 C      -4.462925    -4.591078    -0.764543     115.92
 O      -4.192093    -5.328986    -1.856250     324.61
 H      -5.065699    -5.205499    -2.422899      30.23
 H      -5.431875    -4.114672    -0.665800      28.32
 H      -4.466895    -5.244763     0.077867      26.99
55
name = lig-etoh-frame_135
 C       3.005451     1.745632    -1.763261     105.64
 H       2.720148     2.578974    -2.385952      30.31
 C       3.686903     0.915951     0.236494      67.31
 H       3.702795     0.627718     1.199636      23.56
 C       4.203820    -0.235321    -0.328504      13.78
 O       5.007148    -1.134031     0.432458     216.89
 C       5.512811    -0.634090     1.710298     105.73
 H       4.764008    -0.836249     2.599458      25.63
 H       5.647697     0.463677     1.700941      27.20
 H       6.527714    -1.250166     1.916165      25.20
 C       4.015188    -0.510462    -1.654578      32.76
 O       4.187942    -1.716163    -2.206526     191.93
 H       4.930136    -2.360448    -1.757908      22.93
 C       3.567216     0.578354    -2.392627      60.17
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 H       3.167771     0.341767    -3.461582      17.29
 C       3.057767     1.881609    -0.498565      40.04
 C       2.270801     3.087139     0.159899      85.60
 H       2.619578     4.062543    -0.542393      19.63
 O       2.686084     3.477476     1.529377     240.12
 H       3.665460     3.908691     1.369822      24.74
 C       0.747209     3.047779    -0.207763      57.16
 H       0.492738     3.107804    -1.221167      17.58
 C      -0.088493     4.303736     0.267826      88.73
 O       0.698244     5.483087    -0.382187     144.62
 H       1.017379     4.921212    -1.266185      29.09
 H      -0.211217     4.479592     1.395868      23.99
 H      -1.132207     4.315935    -0.232121      22.80
 C      -1.140191    -1.547203    -0.769654      51.89
 H      -0.566518    -2.357891    -0.652335      20.69
 C      -2.924397    -0.010790    -0.882011      59.70
 H      -4.147802     0.050166    -1.141057      22.81
 C      -2.274565     1.115557    -0.295359       8.56
 O      -2.727364     2.350072    -0.175101     237.72
 C      -4.249480     2.414683    -0.185316     124.47
 H      -4.509696     1.727372    -0.943896      27.05
 H      -4.722416     2.066856     0.796114      26.50
 H      -4.775184     3.347801    -0.024127      25.04
 C      -0.825497     0.771946     0.013860      11.84
 O       0.147281     1.768119     0.494495     162.40
 C      -0.319706    -0.544225    -0.161783      36.05
 H       0.832117    -0.838373     0.302622      15.63
 C      -2.483757    -1.286948    -1.043269      33.48
 C      -3.393007    -2.475841    -1.528561      77.54
 H      -4.289509    -1.978698    -1.767018      25.75
 O      -2.786958    -3.130063    -2.611497     296.80
 H      -2.949765    -3.999399    -2.749867      25.61
 C      -3.600384    -3.455453    -0.303227      97.32
 H      -2.560234    -3.602590     0.009696      22.79
 O      -4.376174    -2.804729     0.756400     342.27
 H      -3.767228    -2.424294     1.368449      28.04
 C      -4.451747    -4.614936    -0.669775     104.04
 O      -4.215357    -5.330857    -1.863306     286.22
 H      -4.880053    -5.043810    -2.551953      31.14
 H      -5.532375    -4.228187    -0.941063      24.39
 H      -4.525451    -5.419943     0.202516      24.55
55
name = lig-etoh-frame_136
 C       3.040489     1.761857    -1.900317      45.06
 H       2.666478     2.614157    -2.484058      18.62
 C       3.703365     0.930740     0.237588      62.75
 H       3.370966     0.761529     1.392390      19.17
 C       4.212075    -0.228988    -0.277874      43.49
 O       4.968193    -1.149277     0.392390     232.26
 C       5.503654    -0.634321     1.699102     121.04
 H       4.720120    -1.058482     2.367166      26.44
 H       5.743173     0.429867     1.777062      27.52
 H       6.374558    -1.156325     1.798752      29.31
 C       4.063225    -0.580016    -1.564532      35.88
 O       4.232322    -1.717794    -2.204190     240.93
 H       4.811815    -2.362322    -2.053833      27.65
 C       3.514790     0.547901    -2.449853     100.41
 H       3.559716     0.481686    -3.540062      25.38
 C       3.075904     1.905113    -0.421929      49.41
 C       2.289203     3.045905     0.179894     118.79
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 H       2.525235     3.893119    -0.316709      24.06
 O       2.692319     3.467440     1.513719     316.75
 H       3.548700     3.776077     1.326698      30.89
 C       0.663455     3.053058    -0.138327      57.90
 H       0.526457     3.009216    -1.237933      17.91
 C      -0.047387     4.288081     0.263432     110.34
 O       0.693646     5.485876    -0.363261     231.86
 H       0.916238     4.979495    -1.080921      36.37
 H      -0.098787     4.422924     1.338620      25.85
 H      -0.914926     4.175198    -0.316274      25.17
 C      -1.111301    -1.503158    -0.767015      37.77
 H      -0.646269    -2.648053    -0.838049      19.78
 C      -2.969625    -0.010837    -0.896872      70.03
 H      -3.973095     0.004845    -0.920219      24.72
 C      -2.273631     1.048924    -0.329829       7.41
 O      -2.772005     2.326856    -0.110737     242.62
 C      -4.208158     2.412960    -0.210693     114.29
 H      -4.830721     1.853634    -1.007430      25.90
 H      -4.621276     1.877598     0.803053      24.67
 H      -4.748313     3.407834    -0.088129      25.45
 C      -0.792440     0.890581    -0.023717      -3.53
 O       0.149951     1.692952     0.523085     157.84
 C      -0.265254    -0.575012    -0.113696      20.64
 H       0.705384    -0.848170     0.024608      19.07
 C      -2.439221    -1.272012    -1.049133      41.97
 C      -3.398305    -2.390722    -1.576655      66.19
 H      -4.607616    -2.140863    -1.705869      22.54
 O      -2.764605    -3.167328    -2.575101     240.31
 H      -3.007435    -4.174258    -2.754088      19.94
 C      -3.626592    -3.381021    -0.320125     100.06
 H      -2.647525    -3.702069     0.097371      23.14
 O      -4.364013    -2.856756     0.758658     331.22
 H      -3.902086    -2.245036     1.422146      26.09
 C      -4.521005    -4.656800    -0.555749     105.33
 O      -4.212111    -5.357588    -1.915677     286.31
 H      -4.669629    -4.956365    -2.606302      33.65
 H      -5.456466    -4.276284    -0.770824      27.43
 H      -4.551240    -5.448279     0.237742      26.68
55
name = lig-etoh-frame_137
 C       3.092301     1.762893    -2.013654      44.77
 H       2.650871     2.513857    -2.678447      19.98
 C       3.689718     0.925054     0.364533      53.01
 H       3.334019     1.188320     1.301852      20.69
 C       4.252609    -0.251654    -0.229174      27.33
 O       4.956314    -1.164359     0.393730     227.36
 C       5.462959    -0.676792     1.663230     104.40
 H       4.797745    -1.057843     2.445824      25.67
 H       5.669391     0.427323     1.670618      25.09
 H       6.518174    -1.332183     1.821742      24.42
 C       4.056137    -0.537441    -1.584634      19.48
 O       4.263848    -1.754212    -2.246109     186.25
 H       5.032955    -2.477256    -1.999426      22.20
 C       3.476127     0.508862    -2.485004      74.83
 H       3.863701     0.474949    -3.543490      27.37
 C       3.052415     1.953710    -0.419891      27.14
 C       2.274882     3.026228     0.192007     101.46
 H       2.542010     4.017367    -0.521769      21.60
 O       2.667452     3.429250     1.503400     256.57
 H       3.665904     3.835296     1.475506      26.79
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 C       0.644140     2.981763    -0.045764      61.94
 H       0.636532     2.582140    -1.100453      18.23
 C      -0.004051     4.305422     0.252438     110.83
 O       0.674798     5.462076    -0.315218     191.49
 H       0.968182     5.223148    -1.329120      28.53
 H      -0.095972     4.429931     1.336678      26.02
 H      -1.079824     4.202403    -0.202962      23.37
 C      -1.030944    -1.526342    -0.732868      45.56
 H      -0.933152    -2.476290    -1.052938      21.49
 C      -3.022270     0.001691    -0.884027      41.16
 H      -4.219179     0.103268    -0.862344      21.42
 C      -2.172127     0.999084    -0.346067       5.81
 O      -2.828110     2.321608    -0.064470     197.69
 C      -4.232667     2.391747    -0.186221     113.11
 H      -4.780973     2.147763    -1.114497      27.35
 H      -4.475811     1.673281     0.648376      25.73
 H      -4.293959     3.493179    -0.240478      25.47
 C      -0.774442     0.898284    -0.079854      24.03
 O       0.154217     1.672243     0.557476     178.29
 C      -0.298512    -0.521835    -0.110342      25.00
 H       0.979331    -0.782125    -0.166822      17.32
 C      -2.426583    -1.288200    -1.101795      14.43
 C      -3.432222    -2.358747    -1.551182      87.83
 H      -4.382917    -2.096019    -1.878759      24.95
 O      -2.720268    -3.194053    -2.583286     225.07
 H      -3.194963    -4.109235    -2.336064      18.05
 C      -3.626970    -3.344288    -0.312163     102.53
 H      -2.695722    -3.820717     0.031229      23.44
 O      -4.376713    -2.880571     0.787398     303.98
 H      -3.843880    -2.137674     1.312713      25.29
 C      -4.579934    -4.688552    -0.525546      71.26
 O      -4.195994    -5.398191    -1.944149     209.57
 H      -4.651348    -4.775101    -2.663389      27.80
 H      -5.718566    -4.240625    -0.420963      25.38
 H      -4.462140    -5.452713     0.281357      26.64
55
name = lig-etoh-frame_138
 C       3.126684     1.759015    -2.020829      56.79
 H       2.742277     2.399521    -2.817541      20.02
 C       3.632781     0.968695     0.446840      37.87
 H       3.582286     1.326361     1.578217      18.89
 C       4.247800    -0.238311    -0.224625       0.89
 O       4.978799    -1.209482     0.439773     214.56
 C       5.466727    -0.774820     1.641043     124.40
 H       4.865480    -0.870945     2.660051      25.65
 H       5.544650     0.295724     1.530897      26.94
 H       6.301881    -1.251851     1.832978      29.66
 C       4.020608    -0.459629    -1.662393      11.79
 O       4.305878    -1.808228    -2.297578     164.79
 H       5.088161    -2.153645    -1.713101      23.52
 C       3.491770     0.467879    -2.500907      72.58
 H       3.888526     0.298339    -3.542076      25.14
 C       3.051073     1.921488    -0.526962      29.19
 C       2.245850     3.092705     0.160858     112.20
 H       2.390327     3.816027    -0.542896      27.76
 O       2.645595     3.384111     1.510781     298.96
 H       3.510945     3.862475     1.584922      28.72
 C       0.708236     2.838617     0.013696      81.34
 H       0.674919     2.569303    -1.021544      21.85
 C      -0.017496     4.317091     0.226036     111.75
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 O       0.667916     5.423161    -0.277719     221.98
 H       0.777954     5.588605    -1.293644      28.90
 H      -0.056181     4.519697     1.349693      25.91
 H      -1.070171     4.354582     0.071234      26.55
 C      -1.040425    -1.538863    -0.715848      35.59
 H      -0.679783    -2.610352    -1.156213      18.40
 C      -3.046963    -0.018795    -0.848850      41.18
 H      -4.104669     0.269743    -0.949544      18.85
 C      -2.113744     1.034421    -0.349556       1.53
 O      -2.817229     2.284159    -0.046236     162.31
 C      -4.260619     2.391282    -0.168567     101.86
 H      -4.541305     2.222133    -1.279206      25.08
 H      -4.816370     1.734249     0.651334      24.56
 H      -4.125467     3.512380    -0.010022      24.04
 C      -0.752824     0.806707    -0.120954      32.63
 O       0.149736     1.696006     0.620217     203.29
 C      -0.280258    -0.455487    -0.173634      46.26
 H       0.671577    -0.482446    -0.081666      23.56
 C      -2.453365    -1.259076    -1.145039      10.54
 C      -3.399808    -2.385006    -1.497401      77.26
 H      -4.262300    -1.784813    -2.166592      21.79
 O      -2.701376    -3.219538    -2.574230     240.07
 H      -2.998098    -4.040239    -2.236235      24.60
 C      -3.660236    -3.383663    -0.297964      88.14
 H      -2.630430    -3.747074    -0.112488      24.18
 O      -4.387175    -2.859756     0.839246     328.50
 H      -3.799704    -2.251765     1.196305      31.46
 C      -4.639211    -4.684011    -0.555483      91.44
 O      -4.206403    -5.409916    -1.938164     273.30
 H      -4.692262    -4.832070    -2.588113      30.76
 H      -5.599820    -4.476138    -0.335676      27.88
 H      -4.178917    -5.449217     0.224923      25.67
55
name = lig-etoh-frame_139
 C       3.142961     1.724479    -1.969261      40.52
 H       2.817484     2.451298    -2.719709      22.53
 C       3.580491     1.003396     0.437439      55.10
 H       3.954451     1.161588     1.425747      23.52
 C       4.188448    -0.185429    -0.232586     -16.00
 O       4.978693    -1.277742     0.457785     176.05
 C       5.465401    -0.829928     1.689382     111.96
 H       4.806721    -0.853599     2.531565      27.29
 H       5.698660     0.276824     1.531768      27.19
 H       6.573386    -1.377545     1.932728      24.96
 C       4.008927    -0.470583    -1.692168       4.84
 O       4.361221    -1.813775    -2.306269     196.99
 H       4.980251    -1.970620    -1.650962      27.29
 C       3.539964     0.473350    -2.539497      52.53
 H       3.568874     0.191735    -3.590858      21.25
 C       3.053639     1.865946    -0.621460      41.08
 C       2.228932     3.116063     0.113962     111.73
 H       2.302912     4.098844    -0.610054      22.83
 O       2.609046     3.336880     1.522885     292.48
 H       3.437726     3.883398     1.489218      27.98
 C       0.774994     2.743029     0.011179      75.35
 H       0.638964     2.779683    -1.133575      19.13
 C      -0.046578     4.286175     0.247050     100.36
 O       0.679364     5.424523    -0.251980     219.03
 H       0.461507     5.522166    -1.137325      33.05
 H       0.119310     4.491255     1.264594      26.88
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 H      -1.172215     4.356758     0.028982      25.10
 C      -1.099808    -1.552978    -0.747154      52.79
 H      -0.395731    -2.314551    -0.863138      18.97
 C      -2.981068    -0.004015    -0.799449      55.14
 H      -4.025918     0.267302    -1.067019      17.92
 C      -2.168892     1.084184    -0.361512      17.06
 O      -2.749838     2.217944    -0.025248     174.55
 C      -4.249875     2.418225    -0.157350     113.93
 H      -4.387177     2.282728    -1.221594      25.79
 H      -5.147078     2.018741     0.414517      25.07
 H      -4.489646     3.399068     0.276857      26.08
 C      -0.745786     0.790029    -0.110272      18.18
 O       0.120422     1.709621     0.706688     192.08
 C      -0.273296    -0.471374    -0.298223      21.66
 H       0.963668    -0.392653     0.212209      16.93
 C      -2.456043    -1.242632    -1.133654      26.07
 C      -3.357578    -2.400384    -1.511126      91.23
 H      -4.081082    -1.890098    -1.982707      26.78
 O      -2.696459    -3.225579    -2.544723     212.70
 H      -2.629763    -4.338704    -2.374356      18.85
 C      -3.748999    -3.447686    -0.301543      78.31
 H      -2.674442    -3.666695    -0.096325      23.31
 O      -4.382863    -2.829490     0.882901     294.87
 H      -3.654479    -2.237255     1.374729      23.17
 C      -4.576759    -4.700958    -0.614858     101.81
 O      -4.251001    -5.392026    -1.893059     320.26
 H      -4.732009    -5.008529    -2.593734      35.05
 H      -5.787238    -4.647704    -0.451842      24.55
 H      -4.200852    -5.341096     0.052094      28.81
55
name = lig-etoh-frame_140
 C       3.145043     1.669272    -1.963275      67.61
 H       2.802912     2.579318    -2.460999      24.76
 C       3.589423     0.955771     0.312544      69.43
 H       4.021311     1.197565     1.301355      22.72
 C       4.121187    -0.165249    -0.249509      -1.55
 O       4.945213    -1.320784     0.438631     178.61
 C       5.538430    -0.850048     1.757306     116.08
 H       4.625373    -1.008742     2.486707      24.22
 H       5.954991     0.138454     1.708236      28.29
 H       6.312541    -1.422620     1.985193      29.79
 C       4.019927    -0.553394    -1.678614       3.03
 O       4.409010    -1.760924    -2.280378     150.38
 H       5.104630    -2.224464    -1.519089      21.12
 C       3.592246     0.505095    -2.590896      53.66
 H       3.104770     0.255236    -3.628521      19.23
 C       3.039327     1.879174    -0.588011      25.35
 C       2.249042     3.101854     0.042427     112.00
 H       2.286590     4.108676    -0.296660      21.99
 O       2.568846     3.291668     1.509824     278.65
 H       3.461259     3.877015     1.416489      26.23
 C       0.773751     2.761379    -0.065982      67.40
 H       0.547882     2.651625    -1.094230      21.20
 C      -0.062582     4.224806     0.307662      86.27
 O       0.690299     5.440224    -0.242557     148.61
 H       0.151382     5.394959    -1.178682      27.13
 H       0.150999     4.283655     1.438778      23.90
 H      -1.060384     4.184126    -0.104516      24.49
 C      -1.111459    -1.517020    -0.781315      44.04
 H      -0.451213    -2.467512    -0.681910      15.38
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 C      -2.905471     0.032636    -0.772269      58.60
 H      -4.015745     0.112104    -1.174692      18.27
 C      -2.201625     1.065571    -0.365892      29.31
 O      -2.713471     2.206277     0.032084     205.47
 C      -4.224238     2.479680    -0.155489     109.04
 H      -4.455604     2.482503    -1.253364      26.21
 H      -4.951283     1.716439     0.324432      25.24
 H      -4.582317     3.432268     0.288635      26.46
 C      -0.771697     0.852203    -0.063609      -3.92
 O       0.075251     1.703149     0.778600     198.24
 C      -0.214215    -0.490518    -0.390952      30.02
 H       0.582895    -0.709047     0.069710      19.69
 C      -2.415752    -1.288367    -1.077899      32.56
 C      -3.314187    -2.452537    -1.530961      75.77
 H      -4.444528    -2.036552    -1.950305      22.35
 O      -2.678717    -3.239978    -2.525945     278.58
 H      -2.474876    -4.138941    -2.407515      25.15
 C      -3.816362    -3.446894    -0.305591      82.65
 H      -2.855016    -3.833563     0.078935      22.43
 O      -4.361857    -2.792455     0.913557     341.96
 H      -3.639724    -2.437536     1.528881      25.54
 C      -4.534022    -4.724724    -0.694904     119.25
 O      -4.294661    -5.373593    -1.839548     293.63
 H      -4.832288    -5.114431    -2.696856      31.64
 H      -5.560845    -4.624074    -0.679589      25.70
 H      -4.299411    -5.537535     0.230417      25.08
55
name = lig-etoh-frame_141
 C       3.118499     1.660991    -1.959332      71.81
 H       2.734900     2.551728    -2.473542      24.65
 C       3.638450     0.902910     0.199759      51.54
 H       3.753009     1.321197     1.247976      20.32
 C       4.110069    -0.275806    -0.317261      19.75
 O       4.907606    -1.302882     0.421944     176.97
 C       5.551405    -0.879947     1.796934      99.01
 H       4.822111    -0.977398     2.509374      26.81
 H       6.094399     0.127390     1.870359      26.38
 H       6.314327    -1.853023     2.108684      24.58
 C       4.025126    -0.592297    -1.680831      25.12
 O       4.479216    -1.708075    -2.210353     224.09
 H       4.898127    -2.409270    -1.744096      26.47
 C       3.609590     0.492850    -2.618561      60.92
 H       3.095041     0.401558    -3.507577      21.69
 C       3.025245     1.929581    -0.521516      20.88
 C       2.273820     3.034413     0.025652     110.88
 H       2.432763     4.129620    -0.386944      19.56
 O       2.544033     3.253209     1.469383     323.78
 H       3.363907     3.693168     1.562648      31.30
 C       0.698551     2.855148    -0.139529      36.70
 H       0.441730     2.356463    -1.158384      18.70
 C      -0.005733     4.135377     0.385224      97.34
 O       0.657602     5.433150    -0.248065     166.34
 H       0.247639     5.458988    -1.165104      28.89
 H      -0.114910     4.077432     1.437032      26.50
 H      -1.010305     4.027331    -0.074246      23.54
 C      -1.024652    -1.510546    -0.805626      40.24
 H      -0.989071    -2.618701    -0.716358      18.66
 C      -2.912278    -0.038057    -0.830812      56.18
 H      -3.890293     0.106664    -1.071782      22.55
 C      -2.133877     1.051636    -0.323872      11.77
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 O      -2.734419     2.277227     0.109338     188.66
 C      -4.203285     2.513055    -0.157662     106.32
 H      -4.492285     2.729994    -1.234244      26.81
 H      -4.337147     1.424097     0.150695      21.99
 H      -4.329501     3.490960     0.327018      25.24
 C      -0.770210     0.866074    -0.012107      16.69
 O       0.028291     1.700697     0.808057     164.17
 C      -0.236734    -0.426413    -0.451578      36.71
 H       0.790418    -1.111805     0.050739      15.92
 C      -2.409562    -1.336202    -1.016085       7.89
 C      -3.352939    -2.513762    -1.518298      94.96
 H      -4.244885    -2.263996    -1.872247      24.65
 O      -2.648831    -3.223587    -2.538964     271.06
 H      -2.489844    -4.151608    -2.186278      22.36
 C      -3.787862    -3.413591    -0.277499      98.88
 H      -2.930933    -3.985227     0.151366      20.31
 O      -4.353866    -2.763857     0.922149     336.46
 H      -3.622347    -2.638526     1.515744      27.16
 C      -4.555077    -4.754012    -0.676551     106.10
 O      -4.298868    -5.399162    -1.861262     317.64
 H      -4.903061    -5.086717    -2.576949      31.87
 H      -5.749864    -4.379790    -0.696609      25.14
 H      -4.511166    -5.387772     0.068358      30.22
55
name = lig-etoh-frame_142
 C       3.071604     1.696806    -1.936108      82.15
 H       2.659041     2.339590    -2.743183      24.16
 C       3.678102     0.893788     0.163913      51.79
 H       3.567104     1.065974     1.222945      19.28
 C       4.150789    -0.424063    -0.359587      17.75
 O       4.883027    -1.249936     0.431067     192.72
 C       5.573985    -0.961557     1.803708     101.78
 H       4.804110    -0.826797     2.730480      24.97
 H       6.118631    -0.054394     1.831461      27.55
 H       6.045911    -1.841516     1.938695      28.15
 C       4.019291    -0.561313    -1.712624      38.27
 O       4.554302    -1.699534    -2.191163     231.40
 H       4.752937    -2.482016    -1.656701      25.36
 C       3.591097     0.478978    -2.559163      53.81
 H       3.347678     0.355514    -3.730248      18.61
 C       3.047291     1.903922    -0.550228      38.58
 C       2.265370     3.015996     0.053263     116.48
 H       2.614831     3.788277    -0.683866      24.01
 O       2.503874     3.204322     1.429273     292.16
 H       3.449664     3.609134     1.633203      27.76
 C       0.636527     2.922075    -0.181625      41.71
 H       0.411983     2.461161    -1.111357      22.10
 C       0.039232     4.059478     0.386069     108.38
 O       0.603163     5.400963    -0.224454     195.85
 H       0.421046     5.425915    -1.140877      31.85
 H      -0.204287     4.068873     1.502835      25.09
 H      -1.038929     4.045942     0.065722      23.45
 C      -1.004447    -1.540419    -0.836302      45.11
 H      -0.887261    -2.619524    -0.820231      20.42
 C      -2.921058    -0.110145    -0.898532      40.87
 H      -4.101065     0.213051    -1.000978      22.57
 C      -2.086117     1.063163    -0.261157     -13.57
 O      -2.730113     2.362873     0.163568     169.23
 C      -4.127074     2.513540    -0.166224     117.02
 H      -4.382331     2.798567    -1.198230      27.36
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 H      -4.515147     1.551451     0.114847      26.26
 H      -4.300344     3.315002     0.601206      25.67
 C      -0.731458     0.830122     0.039117      11.04
 O      -0.010941     1.714916     0.800922     147.19
 C      -0.211435    -0.412423    -0.434767      47.59
 H       0.709145    -0.646012    -0.222466      21.41
 C      -2.437484    -1.363303    -0.980107       9.61
 C      -3.363877    -2.557128    -1.439028      59.59
 H      -4.386671    -2.101863    -2.039688      19.88
 O      -2.614579    -3.222064    -2.558033     193.57
 H      -2.566064    -4.186236    -2.020147      19.23
 C      -3.701450    -3.438714    -0.227603     108.46
 H      -2.747845    -3.892570     0.094220      22.49
 O      -4.356217    -2.742679     0.896015     293.70
 H      -3.544181    -2.711862     1.597083      22.98
 C      -4.691484    -4.696040    -0.630268      91.77
 O      -4.283018    -5.446075    -1.920849     310.03
 H      -4.883502    -5.045631    -2.502218      32.73
 H      -5.615932    -4.245290    -0.664177      27.79
 H      -4.627801    -5.537320     0.290100      25.31
55
name = lig-etoh-frame_143
 C       3.031380     1.701307    -1.984846      58.46
 H       2.551616     2.241107    -2.787630      21.97
 C       3.712864     0.838409     0.172495      63.19
 H       3.532668     0.670748     1.296350      19.98
 C       4.172736    -0.406610    -0.320448      19.27
 O       4.886505    -1.230027     0.469640     209.65
 C       5.512942    -1.021296     1.791182     102.06
 H       4.878404    -0.769931     2.566436      27.34
 H       6.282514    -0.168439     1.637898      25.68
 H       6.105580    -2.087381     1.848228      24.07
 C       4.039463    -0.552717    -1.749342      16.59
 O       4.643429    -1.731979    -2.239481     158.59
 H       4.511638    -2.378095    -1.337493      20.39
 C       3.529871     0.493365    -2.503757      69.64
 H       3.815894     0.287921    -3.491586      25.28
 C       3.069259     1.819309    -0.612637      69.76
 C       2.236620     2.992424     0.044784     130.87
 H       2.568062     3.783548    -0.695147      26.06
 O       2.471422     3.169613     1.411379     297.99
 H       3.417722     3.524493     1.468572      29.56
 C       0.668169     2.889633    -0.172040      46.25
 H       0.355688     2.772524    -1.277969      21.95
 C      -0.017619     4.095532     0.358927     110.13
 O       0.541332     5.352400    -0.159778     192.49
 H       0.626500     5.173730    -1.257891      27.70
 H       0.171069     4.169354     1.440813      26.50
 H      -1.060609     4.114793     0.133597      25.09
 C      -1.037431    -1.560460    -0.850557      42.21
 H      -0.261896    -2.460640    -0.980774      19.25
 C      -2.950834    -0.044615    -0.905018      47.25
 H      -3.928084     0.060771    -1.010332      28.41
 C      -2.116409     1.054501    -0.220147     -21.10
 O      -2.674997     2.399739     0.186875     165.15
 C      -4.045126     2.511403    -0.129868     124.03
 H      -4.197423     2.893866    -1.203890      26.33
 H      -5.010502     1.793063     0.072196      24.65
 H      -4.560213     3.081275     0.679994      25.89
 C      -0.722383     0.787644     0.073143       7.99
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 O      -0.021962     1.751046     0.770959     154.50
 C      -0.206471    -0.441663    -0.404275      11.32
 H       1.152881    -0.244799    -0.348360      16.25
 C      -2.454950    -1.404990    -0.977285       9.35
 C      -3.378815    -2.530094    -1.395377      83.56
 H      -4.149381    -2.086503    -1.809588      24.74
 O      -2.600669    -3.248438    -2.528602     236.60
 H      -2.544350    -4.136181    -2.385880      26.33
 C      -3.634833    -3.519587    -0.187511      94.52
 H      -2.585948    -3.782093     0.082926      23.07
 O      -4.327631    -2.737819     0.860335     320.47
 H      -3.767567    -2.532531     1.619113      27.53
 C      -4.765096    -4.655068    -0.559562      77.78
 O      -4.280771    -5.473643    -1.941227     208.72
 H      -4.858271    -5.004912    -2.687123      27.70
 H      -5.836265    -4.113328    -0.728493      25.84
 H      -4.779545    -5.373860     0.152574      27.53
55
name = lig-etoh-frame_144
 C       2.996187     1.669367    -2.068328      29.77
 H       2.434129     2.441457    -2.640302      19.43
 C       3.709521     0.766139     0.227494      58.44
 H       3.584280     0.725405     1.260376      22.59
 C       4.198549    -0.295633    -0.299710      21.54
 O       4.896085    -1.261908     0.501584     233.63
 C       5.485998    -1.081054     1.724609     127.75
 H       4.748406    -0.786786     2.588100      25.87
 H       6.251855    -0.369455     1.625417      28.75
 H       5.994634    -2.014676     1.986726      27.22
 C       4.099247    -0.578727    -1.726628      15.98
 O       4.710103    -1.770997    -2.276956     220.98
 H       4.552628    -2.223849    -1.503944      28.29
 C       3.504896     0.470233    -2.482167      77.09
 H       4.034761     0.361887    -3.509788      26.58
 C       3.049142     1.752708    -0.631953      50.92
 C       2.202237     2.927876    -0.018544     126.07
 H       2.357833     4.027818    -0.407934      23.49
 O       2.458060     3.148924     1.405252     306.18
 H       3.335605     3.494219     1.406404      32.00
 C       0.704362     2.812949    -0.156886      71.29
 H       0.431535     2.939966    -1.206601      22.12
 C      -0.077070     4.186111     0.360976     107.89
 O       0.489035     5.305670    -0.137690     268.14
 H       0.818321     5.066642    -0.975746      33.37
 H       0.403206     4.214855     1.360941      24.68
 H      -1.230436     4.073174     0.234312      23.35
 C      -0.993279    -1.560190    -0.841686      38.53
 H      -0.244833    -2.170334    -1.187203      22.74
 C      -2.919598     0.044825    -0.843891      43.39
 H      -4.120668     0.051117    -1.082809      25.16
 C      -2.182999     1.020316    -0.196563       7.16
 O      -2.608262     2.359960     0.196201     191.87
 C      -4.048969     2.536689    -0.080651     127.54
 H      -4.047766     3.019586    -1.033920      28.18
 H      -4.689131     1.706581    -0.177367      28.06
 H      -4.543872     3.274583     0.588439      27.47
 C      -0.773419     0.757522     0.082251      -4.18
 O      -0.001354     1.801007     0.711168     187.23
 C      -0.159182    -0.457203    -0.358411      33.33
 H       0.763143    -0.308144    -0.564392      22.93
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 C      -2.430198    -1.402690    -0.984654       4.85
 C      -3.322159    -2.536610    -1.363543      55.11
 H      -4.435875    -2.023916    -1.745685      20.88
 O      -2.604847    -3.246734    -2.489042     191.21
 H      -2.665392    -4.298748    -2.633897      19.59
 C      -3.618428    -3.580423    -0.167336      91.10
 H      -2.637724    -3.934619     0.187641      23.64
 O      -4.299247    -2.742812     0.821937     326.79
 H      -3.799307    -2.342318     1.583768      27.06
 C      -4.776641    -4.595799    -0.557246      78.19
 O      -4.311628    -5.467165    -1.920259     231.07
 H      -4.661660    -5.088499    -2.767837      29.08
 H      -5.722993    -4.113790    -0.824623      26.50
 H      -4.952022    -5.470962     0.251655      25.13
55
name = lig-etoh-frame_145
 C       2.954864     1.632946    -2.069900      30.66
 H       2.514701     2.523857    -2.519997      18.37
 C       3.620937     0.819685     0.293104      46.75
 H       3.645147     1.091029     1.419234      21.62
 C       4.299124    -0.298771    -0.325683      23.74
 O       4.880063    -1.324423     0.469233     232.82
 C       5.456069    -1.113440     1.709669     122.34
 H       4.752471    -0.859290     2.492786      26.45
 H       6.264451    -0.291294     1.771555      27.13
 H       5.900312    -2.133016     2.146544      25.52
 C       4.170541    -0.588696    -1.679527      20.92
 O       4.752679    -1.766437    -2.306880     190.36
 H       4.802170    -2.526939    -1.571220      23.73
 C       3.563687     0.385949    -2.551817      58.69
 H       3.765538     0.455478    -3.609007      25.89
 C       2.992003     1.727339    -0.634349      28.99
 C       2.176824     2.877997    -0.046948     127.39
 H       2.317623     3.903134    -0.381069      21.64
 O       2.452401     3.119026     1.403827     266.88
 H       3.411810     3.585315     1.485611      27.62
 C       0.663404     2.780034    -0.133794      71.97
 H       0.459200     2.650789    -1.241235      20.45
 C      -0.105987     4.195947     0.422645     103.87
 O       0.459634     5.321759    -0.157409     273.13
 H       0.950245     5.135906    -1.021467      27.70
 H       0.161866     4.143097     1.532992      24.87
 H      -1.128486     4.042818     0.383928      25.73
 C      -0.933483    -1.500139    -0.822796      33.35
 H      -0.504247    -2.451207    -1.451802      18.56
 C      -2.929765     0.029062    -0.777668      66.55
 H      -3.904047     0.211022    -1.079294      26.11
 C      -2.211033     1.017671    -0.148838      16.74
 O      -2.564681     2.271672     0.202365     183.57
 C      -4.054069     2.599835    -0.051885     107.05
 H      -3.994767     3.206496    -1.058317      26.22
 H      -4.302203     1.468042    -0.276576      21.85
 H      -4.318540     3.422501     0.641915      25.37
 C      -0.824155     0.746725     0.080591      11.97
 O       0.023877     1.829600     0.625263     200.78
 C      -0.211174    -0.442924    -0.310832      31.20
 H       1.076427    -0.545254    -0.719349      19.43
 C      -2.355286    -1.327821    -0.984441       2.43
 C      -3.286973    -2.576927    -1.366279      85.60
 H      -4.219640    -2.310376    -1.556552      25.35
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 O      -2.604361    -3.233548    -2.457990     223.17
 H      -3.119169    -4.166808    -2.557228      19.93
 C      -3.636374    -3.590385    -0.158175     104.02
 H      -2.843633    -4.225754     0.272155      24.41
 O      -4.287407    -2.753136     0.798207     340.39
 H      -3.537456    -2.256127     1.388611      24.61
 C      -4.724600    -4.589394    -0.607553      94.11
 O      -4.349782    -5.446150    -1.858213     305.28
 H      -4.605125    -5.078293    -2.678026      32.09
 H      -5.667377    -3.987278    -0.892672      26.63
 H      -5.054824    -5.315330     0.137400      27.28
55
name = lig-etoh-frame_146
 C       2.953449     1.530995    -2.005165      59.11
 H       2.664906     2.366917    -2.661697      25.04
 C       3.536463     0.893006     0.319533      59.48
 H       3.704098     1.339940     1.264916      23.31
 C       4.386975    -0.310403    -0.293255      11.18
 O       4.867733    -1.395898     0.397601     199.26
 C       5.451661    -1.133857     1.746817     113.47
 H       4.617066    -0.830989     2.480542      25.09
 H       6.160935    -0.313916     1.832757      27.81
 H       5.787674    -2.153451     2.097160      26.35
 C       4.248006    -0.603558    -1.689402       8.26
 O       4.773199    -1.741608    -2.306919     189.61
 H       5.203122    -2.636757    -1.901954      22.88
 C       3.622878     0.352440    -2.633682      30.53
 H       3.459670     0.239493    -3.757714      20.27
 C       2.915135     1.721402    -0.615456      23.45
 C       2.157669     2.855960    -0.004687     116.82
 H       2.506421     3.751083    -0.761986      21.64
 O       2.469016     3.088185     1.407084     310.66
 H       3.273137     3.605734     1.510177      29.65
 C       0.567733     2.809081    -0.151694      69.37
 H       0.416169     2.408492    -1.179941      21.40
 C      -0.071051     4.125754     0.497771      90.69
 O       0.439194     5.386878    -0.188958     221.42
 H       0.894893     5.160988    -1.148073      25.89
 H      -0.083945     4.152068     1.593321      25.12
 H      -1.247523     4.071714     0.315130      22.94
 C      -0.929767    -1.478833    -0.847522      63.14
 H      -0.845056    -2.436783    -1.195806      24.06
 C      -2.935783    -0.065622    -0.716414      62.93
 H      -3.988010     0.243810    -1.144725      20.76
 C      -2.176241     1.010119    -0.091927      19.53
 O      -2.557867     2.216131     0.216729     198.35
 C      -3.983683     2.668366    -0.074382     121.46
 H      -4.062891     3.159583    -0.981654      28.74
 H      -4.533079     1.699499    -0.053040      25.93
 H      -4.247068     3.178398     0.864957      26.98
 C      -0.812610     0.775631     0.083419      21.30
 O       0.019246     1.787688     0.568024     234.88
 C      -0.188791    -0.426344    -0.309496      52.22
 H       0.792809    -0.615447    -0.314217      23.03
 C      -2.300059    -1.246282    -0.976610      15.84
 C      -3.190648    -2.619176    -1.340980      52.20
 H      -4.400135    -2.280782    -1.650993      21.69
 O      -2.623862    -3.231963    -2.439172     264.27
 H      -3.201866    -3.923526    -2.447298      24.97
 C      -3.646584    -3.594101    -0.162157     103.58
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 H      -2.951928    -4.328702     0.299188      23.19
 O      -4.264936    -2.752776     0.803471     371.37
 H      -3.497268    -2.365457     1.115981      31.78
 C      -4.695493    -4.581729    -0.718372     100.06
 O      -4.379408    -5.420312    -1.765916     316.78
 H      -4.790591    -4.970520    -2.628838      28.29
 H      -5.573547    -3.858252    -0.934359      27.33
 H      -5.030015    -5.259917     0.136959      26.81
55
name = lig-etoh-frame_147
 C       2.989564     1.382484    -1.979475      68.56
 H       2.691327     2.067957    -2.796023      25.66
 C       3.536196     0.884178     0.281182      56.60
 H       3.735267     1.358737     1.278264      21.49
 C       4.398045    -0.267388    -0.253412       4.51
 O       4.895624    -1.447645     0.355293     186.72
 C       5.404339    -1.159265     1.786024     108.59
 H       4.531098    -0.819934     2.380322      25.16
 H       6.190850    -0.351663     1.744810      27.28
 H       5.826502    -2.162848     2.066517      26.37
 C       4.320113    -0.600404    -1.731993      -4.13
 O       4.800811    -1.725788    -2.330588     211.71
 H       5.341148    -2.309143    -1.938084      28.19
 C       3.658534     0.354413    -2.652859      49.36
 H       3.318706    -0.079051    -3.608200      22.05
 C       2.835461     1.696386    -0.577730      33.14
 C       2.136763     2.888877     0.017838     124.16
 H       2.490970     3.574386    -0.713687      22.75
 O       2.478061     3.062714     1.402297     320.19
 H       3.266045     3.683345     1.443847      27.77
 C       0.503662     2.859630    -0.178216      69.94
 H       0.283123     2.710703    -1.255560      21.91
 C      -0.067534     4.068136     0.487367     100.63
 O       0.421357     5.442633    -0.209854     231.49
 H       0.621338     5.149507    -1.038655      33.45
 H       0.005388     4.219773     1.625340      24.68
 H      -1.036172     4.132502     0.162567      25.09
 C      -0.977686    -1.454243    -0.861891      47.81
 H      -0.598888    -2.602921    -0.892255      24.07
 C      -2.957854    -0.093235    -0.642120      66.25
 H      -3.994101     0.026824    -1.066945      20.26
 C      -2.141797     0.929044    -0.079840      14.06
 O      -2.592637     2.228725     0.237443     212.25
 C      -3.890324     2.692833    -0.045168     123.76
 H      -4.126109     3.270533    -1.060844      25.56
 H      -4.908447     1.949308     0.058291      24.29
 H      -4.231003     3.061297     0.935408      25.59
 C      -0.747528     0.797279     0.072686      27.70
 O       0.001499     1.702213     0.581350     219.75
 C      -0.179266    -0.427509    -0.312289      25.09
 H       1.103056    -0.521709     0.125459      17.16
 C      -2.311977    -1.258332    -0.982572      29.35
 C      -3.149290    -2.573720    -1.291991      87.45
 H      -3.980088    -2.154784    -1.639192      26.46
 O      -2.623184    -3.236079    -2.440046     220.52
 H      -3.201365    -4.187349    -2.602621      17.60
 C      -3.631894    -3.611690    -0.192086      96.13
 H      -2.813862    -4.169583     0.282649      24.96
 O      -4.247544    -2.760884     0.815617     313.15
 H      -3.423359    -2.245201     1.221028      24.85
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 C      -4.723441    -4.533131    -0.761610     105.53
 O      -4.398614    -5.401730    -1.731162     329.75
 H      -4.954871    -5.141372    -2.492968      31.12
 H      -5.594671    -3.873916    -1.035476      27.58
 H      -4.982436    -5.122360     0.196442      26.35
55
name = lig-etoh-frame_148
 C       2.992184     1.288121    -1.993536      72.86
 H       2.430021     1.892451    -2.713354      22.32
 C       3.621311     0.806949     0.249184      61.10
 H       3.678771     1.051629     1.326035      19.14
 C       4.359315    -0.233752    -0.293561      21.50
 O       4.952234    -1.452313     0.361052     210.38
 C       5.344464    -1.190059     1.775389     113.36
 H       4.556247    -0.847408     2.405258      26.23
 H       6.173315    -0.436794     1.667971      27.71
 H       5.900369    -2.174426     2.187163      25.46
 C       4.376304    -0.543754    -1.746279      14.67
 O       4.823273    -1.708384    -2.376376     146.00
 H       5.553180    -2.058192    -1.623962      22.54
 C       3.703972     0.291100    -2.577334      48.87
 H       3.421075    -0.020854    -3.539579      21.68
 C       2.783060     1.627878    -0.579852      60.70
 C       2.082783     2.904351     0.007262     111.79
 H       2.451032     3.952924    -0.561781      21.38
 O       2.485154     3.056185     1.392642     282.40
 H       3.279578     3.751751     1.370829      27.25
 C       0.512179     2.886608    -0.182890      73.89
 H       0.147887     3.137736    -1.236475      19.90
 C      -0.079830     4.101352     0.439426      94.82
 O       0.402572     5.466753    -0.195410     163.91
 H       0.434916     5.179429    -1.236939      27.95
 H       0.209105     4.170786     1.439143      26.34
 H      -1.210373     4.128470     0.145779      22.49
 C      -0.950588    -1.475816    -0.838046      41.53
 H      -0.336310    -2.301914    -0.663740      21.89
 C      -2.977560    -0.090159    -0.572279      53.85
 H      -4.062985    -0.048613    -0.795301      22.35
 C      -2.146391     0.874505    -0.097325      12.21
 O      -2.623009     2.234365     0.253145     217.51
 C      -3.886885     2.692349     0.010623     137.55
 H      -3.922469     3.347748    -0.808914      28.75
 H      -4.755331     2.115677    -0.110374      28.07
 H      -4.106094     3.453866     0.846352      26.26
 C      -0.723565     0.737687     0.012188      13.81
 O       0.028614     1.678299     0.644993     174.15
 C      -0.112897    -0.448453    -0.300065      38.89
 H       0.737256    -0.423410     0.266928      17.99
 C      -2.356572    -1.359911    -0.988354      25.71
 C      -3.124728    -2.514742    -1.259773      66.97
 H      -4.147049    -1.867559    -1.668085      21.78
 O      -2.609859    -3.267532    -2.466896     242.64
 H      -2.886033    -4.170411    -2.626171      22.76
 C      -3.587902    -3.573440    -0.228472      93.25
 H      -2.657092    -4.048877     0.159223      24.12
 O      -4.221155    -2.770617     0.839569     310.99
 H      -3.605943    -2.222347     1.442549      25.83
 C      -4.779037    -4.440862    -0.691110      94.12
 O      -4.403790    -5.420298    -1.763360     304.52
 H      -5.031736    -5.438980    -2.465529      33.48
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 H      -5.713625    -3.864891    -1.126449      26.00
 H      -5.094951    -4.993743     0.203172      27.09
55
name = lig-etoh-frame_149
 C       2.907807     1.293935    -1.985277      40.41
 H       2.108248     1.778349    -2.585865      18.67
 C       3.697360     0.740145     0.240384      68.98
 H       3.616111     0.694224     1.318057      21.20
 C       4.349570    -0.294169    -0.382577      17.30
 O       5.002647    -1.414357     0.386465     223.11
 C       5.329612    -1.230051     1.732464     128.34
 H       4.526735    -0.868690     2.526857      25.64
 H       6.076145    -0.436550     1.791685      28.33
 H       5.735912    -2.095903     2.203537      27.96
 C       4.439647    -0.510667    -1.723094      29.81
 O       4.882392    -1.694930    -2.376299     211.46
 H       5.508728    -1.919613    -1.601679      23.57
 C       3.720085     0.233858    -2.511503      49.16
 H       3.722914     0.191694    -3.668997      26.47
 C       2.791098     1.541220    -0.621367      65.03
 C       2.045922     2.931008    -0.043675     118.50
 H       2.298551     3.885342    -0.372262      26.04
 O       2.489916     3.066598     1.381198     288.76
 H       3.223703     3.632436     1.384395      32.72
 C       0.551974     2.914635    -0.169660      84.21
 H       0.203579     2.946883    -1.201049      23.68
 C      -0.126804     4.212711     0.378478     107.36
 O       0.383907     5.443408    -0.192005     244.47
 H       0.314046     5.516749    -1.210627      29.35
 H       0.299834     4.199401     1.465442      25.38
 H      -1.190285     4.054113     0.486320      25.73
 C      -0.879011    -1.498304    -0.772279      42.96
 H      -0.290106    -2.497990    -0.742088      23.52
 C      -2.985353    -0.153646    -0.549363      49.46
 H      -4.163595     0.011420    -0.329479      24.99
 C      -2.166480     0.912243    -0.114338       9.45
 O      -2.604260     2.186759     0.275503     196.12
 C      -3.923094     2.763706     0.078443     112.78
 H      -3.656788     3.481713    -0.878268      24.21
 H      -4.719576     1.874641    -0.181798      23.28
 H      -4.009312     3.622645     0.712011      25.32
 C      -0.745856     0.695744    -0.050967      16.61
 O       0.071172     1.706508     0.700169     124.72
 C      -0.114919    -0.465798    -0.298812      37.19
 H       1.005821    -0.637699     0.327730      16.81
 C      -2.325179    -1.408135    -0.943004      18.81
 C      -3.215171    -2.502340    -1.335887      99.53
 H      -4.113061    -2.131056    -1.541062      26.36
 O      -2.570185    -3.265338    -2.494694     233.61
 H      -2.846251    -4.235011    -2.422872      21.69
 C      -3.542490    -3.469749    -0.239326     101.75
 H      -2.682419    -4.114911    -0.006142      23.59
 O      -4.205762    -2.783734     0.880661     330.67
 H      -3.613676    -2.402325     1.492450      31.13
 C      -4.833849    -4.370566    -0.646988      75.50
 O      -4.394951    -5.435688    -1.787789     229.30
 H      -5.191682    -5.705862    -2.446290      30.07
 H      -5.621481    -3.748595    -1.015049      27.31
 H      -5.296688    -4.967311     0.272513      25.60
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name = lig-etoh-frame_150
 C       2.785889     1.302289    -1.985857      46.18
 H       2.013867     1.720673    -2.605769      21.67
 C       3.719063     0.702145     0.217191      59.77
 H       3.557105     0.521498     1.326074      21.52
 C       4.390224    -0.413768    -0.379872      21.31
 O       5.034992    -1.363812     0.383130     248.38
 C       5.325169    -1.216783     1.730173     119.88
 H       4.499890    -0.974098     2.336148      27.39
 H       6.074459    -0.381936     2.029563      26.37
 H       5.634459    -2.340367     2.157757      24.76
 C       4.512054    -0.556705    -1.741173      22.31
 O       4.973041    -1.672224    -2.333511     235.15
 H       5.547932    -2.192977    -1.784662      25.32
 C       3.653510     0.298492    -2.544692      68.37
 H       4.038940     0.268898    -3.536688      28.76
 C       2.839551     1.498707    -0.622060      43.38
 C       2.054520     2.902210    -0.061447      99.57
 H       2.432181     3.950036    -0.678229      22.02
 O       2.470113     3.068094     1.367524     250.27
 H       3.374522     3.599436     1.389562      27.01
 C       0.553002     2.922486    -0.140482      70.69
 H       0.369612     2.438268    -1.195083      20.43
 C      -0.135715     4.302041     0.377654     115.90
 O       0.360789     5.436145    -0.197754     289.87
 H       0.220903     5.603444    -1.081292      32.36
 H       0.212316     4.395196     1.367002      26.77
 H      -1.232624     4.109467     0.629051      25.01
 C      -0.834982    -1.589460    -0.709267      49.34
 H      -0.586950    -2.612043    -1.047437      20.56
 C      -2.977951    -0.222589    -0.515733      57.42
 H      -3.951070    -0.140852    -0.195119      24.64
 C      -2.186557     0.957588    -0.145322       7.45
 O      -2.568630     2.131593     0.322064     187.32
 C      -3.922822     2.848883     0.058407     113.78
 H      -3.750755     3.225816    -0.870776      28.07
 H      -4.623956     2.006693    -0.034068      26.18
 H      -4.161933     3.492861     0.958321      25.78
 C      -0.756490     0.762381    -0.053359      15.11
 O       0.093225     1.744767     0.711216     150.03
 C      -0.092334    -0.496724    -0.259160      40.13
 H       0.987586    -0.811047    -0.154483      20.17
 C      -2.260279    -1.388001    -0.869169      14.19
 C      -3.277303    -2.538432    -1.451069      57.40
 H      -4.453893    -2.200035    -1.770735      21.55
 O      -2.540393    -3.250715    -2.512364     215.84
 H      -2.918508    -4.221431    -2.157836      19.36
 C      -3.556510    -3.413197    -0.223567     107.09
 H      -2.766379    -4.169019    -0.025682      23.83
 O      -4.186242    -2.797890     0.922541     288.31
 H      -3.355623    -2.569232     1.572691      24.83
 C      -4.853825    -4.359389    -0.634138      55.28
 O      -4.398601    -5.426959    -1.786400     271.20
 H      -5.207443    -5.738903    -2.209500      33.13
 H      -5.605958    -3.470650    -1.017434      25.66
 H      -5.233989    -4.865739     0.175456      27.34
55
name = lig-etoh-frame_151
 C       2.694704     1.266266    -2.011604      43.05
 H       2.039683     1.856195    -2.705546      22.53
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 C       3.704414     0.647941     0.179842      58.09
 H       3.563582     0.747656     1.223354      22.35
 C       4.427724    -0.477312    -0.323646      25.72
 O       5.085559    -1.343875     0.362609     234.23
 C       5.340666    -1.215931     1.785624     127.11
 H       4.307873    -0.999391     2.244154      25.41
 H       6.083276    -0.513975     2.072448      28.45
 H       5.609114    -2.181604     1.970115      28.79
 C       4.512468    -0.579469    -1.782190      13.73
 O       5.090069    -1.662171    -2.313895     195.06
 H       5.555174    -2.567801    -1.924175      20.45
 C       3.619363     0.372430    -2.577835      68.93
 H       4.007271     0.333859    -3.636524      26.07
 C       2.872556     1.518183    -0.573223      41.58
 C       2.135826     2.870685    -0.059413     105.04
 H       2.491200     3.531857    -0.793753      24.25
 O       2.454148     3.083680     1.343032     291.19
 H       3.402492     3.445330     1.362581      27.83
 C       0.529558     2.879029    -0.123583      73.91
 H       0.408034     2.432666    -1.066034      22.32
 C      -0.136221     4.304537     0.408923      96.53
 O       0.351143     5.480568    -0.208629     200.53
 H       0.036856     5.504383    -1.258824      26.73
 H       0.247207     4.493947     1.485583      24.57
 H      -1.259273     4.303532     0.366463      24.39
 C      -0.877304    -1.684237    -0.679793      41.67
 H      -0.593583    -2.605386    -1.191858      18.55
 C      -2.901718    -0.229569    -0.464610      52.48
 H      -4.120856    -0.435879    -0.241833      19.43
 C      -2.173352     0.934622    -0.186579      10.44
 O      -2.564265     2.134083     0.393796     178.16
 C      -3.879190     2.870103     0.055363     110.45
 H      -3.938697     3.312774    -1.066756      24.56
 H      -4.793801     2.081401     0.078861      24.45
 H      -4.225970     3.244972     1.003292      25.85
 C      -0.710496     0.837180    -0.008310      11.02
 O       0.084014     1.776131     0.696804     195.86
 C      -0.098442    -0.530449    -0.242696      15.06
 H       1.138135    -0.660570    -0.365685      19.32
 C      -2.250334    -1.385000    -0.826403      15.18
 C      -3.302508    -2.524554    -1.533154      83.13
 H      -4.106364    -2.161459    -2.020894      26.27
 O      -2.543782    -3.256988    -2.493503     292.90
 H      -2.780965    -4.128608    -2.453592      28.28
 C      -3.648060    -3.452274    -0.227863     105.06
 H      -2.770984    -4.049084     0.076487      25.29
 O      -4.125313    -2.800102     0.978300     324.20
 H      -3.342377    -2.644004     1.527360      28.76
 C      -4.830375    -4.334546    -0.684334      86.93
 O      -4.413477    -5.376982    -1.739001     296.88
 H      -5.236265    -5.696597    -2.075939      34.26
 H      -5.534953    -3.674495    -1.028994      28.27
 H      -5.215687    -4.958236     0.302628      25.14
55
name = lig-etoh-frame_152
 C       2.656792     1.233614    -2.013563      49.18
 H       2.213723     1.989272    -2.653645      24.82
 C       3.661968     0.610448     0.158502      59.18
 H       3.714074     1.057918     1.229123      22.84
 C       4.417722    -0.438454    -0.354428      18.18
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 O       5.183148    -1.374106     0.368378     206.09
 C       5.316673    -1.212558     1.828598     105.94
 H       4.457187    -0.923294     2.383043      25.67
 H       6.199528    -0.477642     2.069344      25.78
 H       5.767781    -2.361645     2.058826      23.81
 C       4.440198    -0.565157    -1.763809      11.47
 O       5.228976    -1.675969    -2.356498     208.63
 H       5.282269    -2.463747    -1.774805      25.19
 C       3.653518     0.380258    -2.609530      56.51
 H       3.582708     0.408165    -3.723092      19.04
 C       2.862421     1.538697    -0.570250      33.20
 C       2.203381     2.784407    -0.021352     106.13
 H       2.610120     3.534887    -0.938409      19.69
 O       2.457393     3.114450     1.311938     333.60
 H       3.362462     3.367409     1.395522      30.07
 C       0.543046     2.843355    -0.102994      63.79
 H       0.194155     2.811755    -1.266004      20.94
 C      -0.120130     4.273385     0.444894      94.11
 O       0.346967     5.548306    -0.255000     230.70
 H       0.051717     5.335470    -1.162871      30.39
 H       0.125134     4.355080     1.481605      26.68
 H      -1.177017     4.309693     0.171564      24.61
 C      -0.939712    -1.708965    -0.665338      43.24
 H      -0.336770    -2.566263    -1.150755      18.32
 C      -2.873915    -0.218463    -0.406139      58.96
 H      -3.841348    -0.342458    -0.473644      20.87
 C      -2.105315     0.923210    -0.177734       2.92
 O      -2.604066     2.171888     0.453994     199.96
 C      -3.848631     2.798073     0.042455     125.92
 H      -3.978908     3.508840    -0.742190      28.24
 H      -4.741569     2.130516     0.008801      26.46
 H      -4.065231     3.453598     0.954760      26.49
 C      -0.652891     0.808664     0.039019       4.46
 O       0.048806     1.791958     0.683462     225.35
 C      -0.111692    -0.552644    -0.244115      17.41
 H       1.007768    -0.266324    -0.423968      18.65
 C      -2.287810    -1.451037    -0.838557      21.20
 C      -3.240404    -2.496548    -1.515167      56.93
 H      -4.033729    -1.843097    -2.246334      21.79
 O      -2.531450    -3.261963    -2.482671     243.74
 H      -2.779261    -4.239054    -2.786287      23.11
 C      -3.746511    -3.505145    -0.260120      78.08
 H      -2.773734    -3.948503     0.001602      24.84
 O      -4.066486    -2.797346     1.022918     315.95
 H      -3.268817    -2.566439     1.534633      25.75
 C      -4.792524    -4.378158    -0.701636     104.93
 O      -4.426775    -5.297503    -1.668329     260.38
 H      -5.320124    -5.691680    -2.068545      30.79
 H      -5.804383    -3.818929    -1.174734      23.94
 H      -5.132428    -4.854922     0.111814      27.38
55
name = lig-etoh-frame_153
 C       2.702887     1.221476    -1.978177      63.50
 H       2.298657     2.043267    -2.597604      24.71
 C       3.600228     0.645563     0.192142      59.44
 H       3.977824     1.003030     1.116777      24.60
 C       4.408105    -0.389749    -0.406203      -3.59
 O       5.271671    -1.395748     0.381275     163.55
 C       5.357651    -1.244391     1.856845     125.54
 H       4.486944    -0.890023     2.530291      25.36
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 H       6.089987    -0.521550     2.019670      28.89
 H       5.664976    -2.096153     2.266059      29.61
 C       4.368267    -0.575688    -1.788906      11.01
 O       5.337869    -1.651067    -2.398473     176.98
 H       5.086704    -2.243314    -1.640311      24.82
 C       3.663500     0.351282    -2.621455      46.62
 H       3.368626     0.271155    -3.661764      21.32
 C       2.830503     1.496522    -0.622568      29.20
 C       2.222081     2.728949    -0.037880     119.25
 H       2.513044     3.596172    -0.582756      22.15
 O       2.472804     3.148257     1.295684     288.93
 H       3.484955     3.450290     1.466660      26.47
 C       0.584801     2.865999    -0.134191      75.65
 H       0.139968     3.088313    -1.043504      22.53
 C      -0.073249     4.242393     0.446711      80.67
 O       0.348188     5.584399    -0.285183     225.36
 H       0.212536     5.352731    -1.199702      31.08
 H      -0.044903     4.293032     1.572633      25.14
 H      -1.194262     4.064762     0.170211      23.39
 C      -0.925957    -1.668195    -0.664995      41.88
 H      -0.331109    -2.475461    -0.917865      19.46
 C      -2.826430    -0.221090    -0.383971      41.72
 H      -4.055459     0.061193    -0.675903      18.36
 C      -2.022896     0.951088    -0.094709       8.87
 O      -2.640128     2.190390     0.478563     185.35
 C      -3.842756     2.738056     0.087354     121.44
 H      -3.711050     3.633495    -0.754529      24.61
 H      -4.689666     1.977666    -0.092199      24.45
 H      -3.925583     3.546273     0.793238      25.58
 C      -0.656104     0.687935     0.069129      19.39
 O       0.010066     1.795427     0.671659     215.96
 C      -0.152076    -0.515927    -0.254803      41.26
 H       1.021561    -0.397033    -0.360681      19.54
 C      -2.330909    -1.527243    -0.864407      24.68
 C      -3.202365    -2.460620    -1.477135      93.44
 H      -3.866042    -1.847717    -1.902500      26.76
 O      -2.478357    -3.275746    -2.491167     224.32
 H      -3.117773    -4.066569    -2.826283      23.37
 C      -3.762126    -3.464864    -0.285762      71.40
 H      -2.847400    -4.107914    -0.244808      23.45
 O      -4.032038    -2.804916     1.043285     276.50
 H      -3.090572    -2.442333     1.429505      21.26
 C      -4.867532    -4.412868    -0.710218     106.34
 O      -4.422406    -5.253973    -1.640081     301.40
 H      -5.189092    -5.653168    -2.072510      33.43
 H      -5.685508    -3.912745    -1.038207      27.78
 H      -5.241697    -4.982507     0.336165      25.21
55
name = lig-etoh-frame_154
 C       2.804091     1.235189    -1.977699      65.70
 H       2.237124     1.939577    -2.585995      24.81
 C       3.592749     0.667995     0.220976      60.23
 H       4.040983     0.917374     1.216444      23.31
 C       4.405469    -0.366456    -0.409104     -17.36
 O       5.318351    -1.385946     0.383613     135.22
 C       5.392292    -1.237012     1.870981     103.07
 H       4.423371    -0.928294     2.323199      24.93
 H       6.181980    -0.384396     2.061836      25.97
 H       5.694253    -2.271237     2.525592      24.23
 C       4.357149    -0.611355    -1.876871      11.80
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 O       5.390667    -1.579466    -2.409968     146.50
 H       5.162998    -2.313406    -1.599081      21.75
 C       3.612409     0.301715    -2.609239      52.34
 H       3.500681    -0.018052    -3.699601      21.04
 C       2.794681     1.439117    -0.636752      36.31
 C       2.173998     2.739298    -0.069766     108.14
 H       2.522214     3.810675    -0.542072      19.19
 O       2.511581     3.165288     1.319413     297.30
 H       3.392194     3.574052     1.324331      28.64
 C       0.645626     2.919926    -0.132705      59.32
 H       0.220226     2.895777    -1.262473      20.84
 C      -0.031903     4.217572     0.430711      93.67
 O       0.342539     5.574949    -0.277630     186.86
 H       0.536887     5.423711    -1.368115      26.01
 H      -0.066513     4.434156     1.517878      25.04
 H      -1.031871     3.931205     0.265819      24.90
 C      -0.896141    -1.585717    -0.669557      41.38
 H      -0.381360    -2.648294    -0.748676      19.57
 C      -2.833279    -0.193633    -0.426542      58.47
 H      -3.678118     0.214043    -0.631221      19.36
 C      -2.031754     0.946140     0.018979      12.47
 O      -2.612080     2.155844     0.495203     213.51
 C      -3.843667     2.748265     0.093173     120.67
 H      -3.495050     3.127550    -0.829867      26.50
 H      -4.667009     1.968783    -0.182831      24.76
 H      -4.185299     3.415169     0.939382      25.72
 C      -0.697018     0.661855     0.118993      24.73
 O      -0.012828     1.789877     0.653959     190.14
 C      -0.149897    -0.510682    -0.288868      54.10
 H       0.958903    -0.943029    -0.119925      19.63
 C      -2.298277    -1.494450    -0.834385      30.60
 C      -3.192740    -2.495047    -1.427387      73.91
 H      -4.199478    -1.837864    -1.823795      23.39
 O      -2.445179    -3.285787    -2.499393     243.01
 H      -3.219133    -3.745156    -2.671283      26.82
 C      -3.723501    -3.407054    -0.296644      72.47
 H      -3.003126    -4.251325    -0.310057      21.57
 O      -3.985869    -2.822612     1.029551     315.08
 H      -3.188057    -2.424857     1.282535      29.55
 C      -4.992270    -4.414472    -0.599012      83.98
 O      -4.387993    -5.261345    -1.671425     318.94
 H      -5.058822    -5.681826    -2.173197      34.75
 H      -5.930695    -3.690752    -0.980412      25.92
 H      -5.179947    -4.941818     0.224054      29.36
55
name = lig-etoh-frame_155
 C       2.886311     1.271134    -2.026168      56.47
 H       2.160180     1.802548    -2.652965      20.06
 C       3.663491     0.637030     0.234826      49.91
 H       3.714229     0.919240     1.317858      19.72
 C       4.411117    -0.381303    -0.394553     -13.28
 O       5.332826    -1.348147     0.375058     156.92
 C       5.436014    -1.218084     1.884506     124.33
 H       4.379334    -0.942223     2.100925      25.54
 H       6.111072    -0.478677     2.171637      29.24
 H       5.684709    -2.102105     2.248651      29.79
 C       4.421013    -0.658528    -1.899016      14.59
 O       5.381526    -1.494421    -2.383900     238.11
 H       5.586997    -2.280737    -1.969529      27.33
 C       3.557129     0.191963    -2.639101      61.11
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 H       3.673413    -0.017969    -3.664882      28.49
 C       2.766694     1.431788    -0.581688      53.06
 C       2.125697     2.839053    -0.083672     108.36
 H       2.517031     3.542256    -0.784129      26.69
 O       2.547888     3.154720     1.349641     275.43
 H       3.393698     3.706189     1.200316      27.14
 C       0.674191     2.942873    -0.158121      67.68
 H       0.560776     2.591964    -1.141431      23.68
 C       0.014781     4.225166     0.385115     101.71
 O       0.342242     5.528630    -0.271944     265.32
 H       0.756121     5.400586    -1.080392      33.41
 H       0.221639     4.529489     1.416803      24.77
 H      -1.143690     3.973690     0.236270      22.82
 C      -0.894695    -1.578149    -0.689961      60.61
 H      -0.573159    -2.547262    -0.671133      23.98
 C      -2.802165    -0.143636    -0.483797      56.12
 H      -4.018999     0.183779    -0.737789      23.68
 C      -2.127867     0.882788     0.119741      22.78
 O      -2.541324     2.092377     0.537456     210.15
 C      -3.844785     2.732815     0.071626     120.29
 H      -3.590845     3.010818    -1.030093      25.71
 H      -4.676651     1.994544    -0.145490      26.56
 H      -4.413736     3.206538     0.867930      26.56
 C      -0.705353     0.753436     0.180198       9.96
 O      -0.004171     1.790266     0.646558     174.41
 C      -0.085930    -0.554163    -0.298318      41.48
 H       0.810849    -0.752224     0.043708      22.06
 C      -2.251556    -1.364075    -0.786087      37.75
 C      -3.225052    -2.507721    -1.386366      83.09
 H      -4.077653    -2.191235    -1.814042      25.28
 O      -2.441478    -3.267836    -2.478945     178.27
 H      -3.343308    -3.857382    -2.800056      19.69
 C      -3.708620    -3.433528    -0.282549      82.42
 H      -2.983180    -4.254353    -0.109474      20.61
 O      -3.945313    -2.847949     0.981714     323.86
 H      -3.132232    -2.321396     1.368121      25.33
 C      -5.087989    -4.330601    -0.537710      70.35
 O      -4.362539    -5.262038    -1.700127     229.85
 H      -5.036379    -5.754595    -2.372315      30.17
 H      -5.919308    -3.851363    -0.826751      27.39
 H      -5.221782    -5.086239     0.430949      24.96
55
name = lig-etoh-frame_156
 C       2.920830     1.290458    -2.049210      39.89
 H       2.208460     1.768786    -2.749102      20.14
 C       3.712547     0.614499     0.233639      53.26
 H       3.468266     0.807812     1.270164      20.67
 C       4.453308    -0.444076    -0.374852      12.28
 O       5.335807    -1.284207     0.350097     186.60
 C       5.432232    -1.169682     1.833399      97.33
 H       4.340053    -0.962864     2.201270      24.19
 H       6.165631    -0.383155     2.310143      25.28
 H       5.775243    -2.335166     2.074787      24.00
 C       4.476587    -0.673051    -1.797800      16.93
 O       5.373808    -1.408063    -2.395432     202.06
 H       5.886343    -2.259118    -2.128810      23.15
 C       3.546656     0.056432    -2.663244      32.89
 H       3.679736     0.156293    -3.820878      26.17
 C       2.779907     1.451590    -0.554153      38.62
 C       2.142471     2.906261    -0.037723     104.63
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 H       2.579063     3.404787    -1.044654      22.98
 O       2.585268     3.142858     1.342561     282.82
 H       3.442058     3.773151     1.310805      26.02
 C       0.664718     2.912959    -0.178562      64.62
 H       0.537617     2.540085    -1.271517      20.27
 C       0.019644     4.254509     0.316774     111.51
 O       0.350387     5.476798    -0.256246     275.30
 H       0.939445     5.274177    -1.079345      29.66
 H       0.539114     4.294617     1.352659      23.85
 H      -0.998233     4.207515     0.308497      26.26
 C      -0.904832    -1.594927    -0.700236      44.56
 H      -0.570506    -2.709857    -0.748465      21.89
 C      -2.882750    -0.063221    -0.557423      81.02
 H      -3.842803    -0.221708    -0.722977      27.37
 C      -2.165680     0.827521     0.188675      13.77
 O      -2.518381     2.071415     0.598265     186.49
 C      -3.835080     2.647023     0.013161     103.59
 H      -3.845720     3.306480    -0.885338      26.59
 H      -4.596028     1.750102    -0.072761      24.96
 H      -4.293475     3.364781     0.760395      26.45
 C      -0.695439     0.785161     0.187132      -1.75
 O       0.043346     1.821368     0.670948     179.39
 C      -0.050758    -0.508173    -0.253677       7.67
 H       1.140879    -0.401340     0.151511      16.53
 C      -2.272020    -1.280049    -0.796143      29.47
 C      -3.199093    -2.510527    -1.345303      59.21
 H      -4.179043    -2.139496    -2.016142      21.19
 O      -2.488615    -3.244727    -2.445165     256.44
 H      -2.890925    -3.989460    -2.860849      26.62
 C      -3.713721    -3.535888    -0.230872      77.81
 H      -2.893803    -4.242202    -0.032463      21.78
 O      -3.915303    -2.846206     0.951377     350.67
 H      -3.144756    -2.367952     1.452933      25.02
 C      -5.063748    -4.296883    -0.495200      74.37
 O      -4.373097    -5.247220    -1.716719     254.97
 H      -4.992171    -5.618030    -2.354082      32.81
 H      -6.158821    -3.847390    -0.856807      24.57
 H      -5.246893    -4.927031     0.292778      27.29
55
name = lig-etoh-frame_157
 C       2.927183     1.233553    -2.040283      39.69
 H       2.397252     1.880699    -2.755154      19.59
 C       3.695836     0.617168     0.198925      44.32
 H       3.514200     0.567673     1.338335      20.61
 C       4.492279    -0.486852    -0.332332      29.87
 O       5.352658    -1.212783     0.332998     246.37
 C       5.412521    -1.157246     1.775114     134.66
 H       4.508864    -1.047135     2.361681      27.26
 H       6.071056    -0.438050     2.167201      28.98
 H       5.762107    -2.090089     1.985868      29.16
 C       4.468681    -0.643192    -1.685237      15.43
 O       5.411712    -1.355751    -2.463310     162.80
 H       5.900025    -2.130667    -1.893851      23.97
 C       3.558434     0.002215    -2.634259      37.35
 H       3.638641     0.101965    -3.669715      27.02
 C       2.855637     1.470974    -0.594037      40.37
 C       2.226588     2.891107    -0.015767     118.80
 H       2.580207     3.603037    -0.699420      26.77
 O       2.625556     3.153272     1.310663     329.82
 H       3.436132     3.607771     1.440145      30.55
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 C       0.617037     2.854517    -0.227267      78.86
 H       0.304318     2.754902    -1.251409      22.21
 C       0.047027     4.242390     0.298329     103.26
 O       0.391808     5.454510    -0.280427     251.64
 H       0.988332     5.248334    -1.145076      27.71
 H       0.465085     4.050111     1.269828      25.39
 H      -1.141653     4.286806     0.523410      23.55
 C      -0.884327    -1.586975    -0.673208      31.95
 H      -0.540411    -2.580511    -0.930136      22.01
 C      -2.965883    -0.031888    -0.616803      50.54
 H      -4.177275    -0.294383    -0.700036      22.72
 C      -2.121154     0.845493     0.207154       0.06
 O      -2.559664     2.103417     0.651261     172.45
 C      -3.837233     2.548132     0.000042     113.02
 H      -3.778557     3.339277    -0.839740      25.59
 H      -4.433029     1.699477    -0.083727      26.74
 H      -4.002905     3.350741     0.724632      25.76
 C      -0.687561     0.725739     0.152518      12.77
 O       0.105652     1.867210     0.714288     192.35
 C      -0.025215    -0.405625    -0.157868      34.46
 H       0.971424    -0.325780    -0.260959      20.66
 C      -2.300441    -1.305037    -0.867963       4.18
 C      -3.205416    -2.519037    -1.359095      76.43
 H      -3.986857    -1.976243    -1.753288      25.32
 O      -2.496733    -3.200804    -2.410666     253.48
 H      -2.764353    -4.120286    -2.640404      25.12
 C      -3.701109    -3.611005    -0.183670      78.87
 H      -2.897223    -4.387092    -0.154622      22.54
 O      -3.916216    -2.816581     0.972380     364.15
 H      -3.106664    -2.560996     1.371517      29.38
 C      -4.992907    -4.298310    -0.544262      90.14
 O      -4.406985    -5.211219    -1.701879     296.25
 H      -5.113588    -5.434661    -2.310544      33.49
 H      -5.819014    -3.775878    -0.848731      27.85
 H      -5.269142    -5.005998     0.399663      25.31
55
name = lig-etoh-frame_158
 C       2.917429     1.136047    -2.023815      86.72
 H       2.615831     1.978821    -2.669839      22.56
 C       3.650671     0.595973     0.185472      58.93
 H       3.691638     0.562696     1.222345      22.87
 C       4.458558    -0.435443    -0.296564      32.54
 O       5.402326    -1.172966     0.350120     251.21
 C       5.398335    -1.149937     1.721930     117.46
 H       4.436012    -1.123646     2.441115      24.67
 H       6.135805    -0.290959     1.986954      26.22
 H       5.933908    -2.185881     2.082331      25.17
 C       4.450173    -0.624576    -1.707127      24.73
 O       5.464167    -1.331087    -2.505194     232.47
 H       5.744255    -1.835214    -1.823834      30.38
 C       3.566038     0.048184    -2.504284      41.69
 H       3.690560    -0.199767    -3.637614      24.66
 C       2.968269     1.502010    -0.664151      42.03
 C       2.314683     2.820757    -0.048101     121.12
 H       2.650813     3.940037    -0.425427      17.12
 O       2.633650     3.152496     1.297222     289.20
 H       3.672225     3.493932     1.363151      25.84
 C       0.575892     2.830945    -0.254186      69.92
 H       0.177684     2.751096    -1.314837      19.73
 C       0.035209     4.177961     0.335850      97.63
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 O       0.466513     5.454067    -0.335699     286.46
 H       0.833962     5.294367    -1.138850      32.84
 H       0.387868     4.179522     1.457087      23.38
 H      -0.974490     4.154817     0.498142      25.72
 C      -0.875383    -1.492283    -0.629577      32.69
 H      -0.397653    -2.419517    -1.038144      20.38
 C      -3.013613    -0.071479    -0.632509      35.33
 H      -4.051119     0.128800    -0.557519      22.91
 C      -2.104828     0.905772     0.148516      -9.34
 O      -2.609580     2.126365     0.681295     184.42
 C      -3.800504     2.517435     0.034420     103.31
 H      -3.467388     2.883921    -0.998321      25.32
 H      -4.639664     1.630233    -0.151468      23.28
 H      -4.169060     3.172543     0.870345      25.15
 C      -0.689058     0.735152     0.165048      12.15
 O       0.145596     1.882561     0.741299     173.87
 C      -0.047109    -0.406214    -0.123505      39.91
 H       1.064421    -0.417308    -0.594397      18.76
 C      -2.299793    -1.372116    -0.937475       4.08
 C      -3.193642    -2.534444    -1.353060      62.15
 H      -4.210161    -1.865057    -1.632843      21.89
 O      -2.479632    -3.158567    -2.404252     196.14
 H      -2.859681    -4.159310    -2.123239      19.98
 C      -3.660391    -3.609714    -0.168936      87.66
 H      -2.946032    -4.445590    -0.132921      24.38
 O      -3.935118    -2.796265     1.010915     328.40
 H      -2.946168    -2.692271     1.404862      24.10
 C      -4.870873    -4.377646    -0.603238      90.76
 O      -4.463076    -5.167048    -1.667444     298.38
 H      -5.302866    -5.211042    -2.315331      28.87
 H      -5.660148    -3.494504    -0.964525      25.19
 H      -5.275520    -4.932256     0.234946      26.82
55
name = lig-etoh-frame_159
 C       2.873437     1.129690    -1.997415      89.10
 H       2.641546     1.911277    -2.706440      27.01
 C       3.610666     0.570541     0.199641      70.61
 H       3.751587     0.902397     1.324625      22.08
 C       4.421670    -0.375900    -0.335204      16.19
 O       5.440969    -1.159026     0.352287     228.59
 C       5.439886    -1.159121     1.758768     131.81
 H       4.457827    -1.124576     2.128575      27.12
 H       5.969886    -0.254034     2.003452      27.85
 H       6.018072    -1.982658     2.096938      27.80
 C       4.471908    -0.634079    -1.766874      21.10
 O       5.486471    -1.300524    -2.508428     178.86
 H       5.912161    -1.896988    -1.696564      23.16
 C       3.590153     0.081616    -2.440500      66.08
 H       3.602808    -0.377334    -3.397325      23.76
 C       3.069795     1.547619    -0.698043      46.00
 C       2.377449     2.801158    -0.134929     111.80
 H       2.638125     3.661323    -0.608530      22.54
 O       2.649998     3.125070     1.315656     338.76
 H       3.554636     3.383813     1.192488      29.65
 C       0.589145     2.847711    -0.239393      52.21
 H       0.254480     2.544335    -1.249411      21.62
 C       0.062709     4.132294     0.395310      86.02
 O       0.534143     5.444386    -0.362724     195.92
 H       0.693113     5.182103    -1.426938      25.11
 H       0.381956     4.420262     1.348884      24.48
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 H      -1.143780     4.022934     0.275037      21.61
 C      -0.899832    -1.399065    -0.614737      47.62
 H      -0.236338    -2.213519    -1.043848      20.74
 C      -2.927852    -0.115187    -0.581245      38.64
 H      -4.009264     0.317450    -0.572105      18.25
 C      -2.126159     0.951646     0.033932      11.31
 O      -2.636518     2.100782     0.704775     237.66
 C      -3.798128     2.495812     0.073418     131.56
 H      -3.440851     2.617692    -0.998569      25.83
 H      -4.589730     1.846546    -0.068887      27.61
 H      -4.494016     3.154357     0.647721      26.22
 C      -0.690818     0.840998     0.235497      -1.05
 O       0.148502     1.850718     0.742037     200.68
 C      -0.063048    -0.477341    -0.170622      32.86
 H       0.967918    -0.501668    -0.485447      21.21
 C      -2.304330    -1.375488    -0.940632      33.91
 C      -3.198863    -2.497456    -1.322018      91.35
 H      -4.167618    -2.265097    -1.610295      25.58
 O      -2.484597    -3.171030    -2.396155     282.36
 H      -2.696187    -4.013089    -2.171974      28.56
 C      -3.595394    -3.555974    -0.167655      91.49
 H      -2.775369    -4.275371     0.123579      23.63
 O      -3.932124    -2.807701     1.042044     355.66
 H      -3.126841    -2.609015     1.579043      26.68
 C      -4.799776    -4.374035    -0.644064     105.38
 O      -4.529660    -5.153598    -1.678232     347.31
 H      -5.213796    -5.083992    -2.335689      32.43
 H      -5.411497    -3.576986    -0.927541      28.40
 H      -5.317857    -4.970121     0.217032      25.74
55
name = lig-etoh-frame_160
 C       2.822564     1.208758    -1.986002      79.92
 H       2.372800     1.784937    -2.831418      23.82
 C       3.590047     0.605216     0.256499      76.86
 H       3.698835     1.093273     1.154781      24.40
 C       4.466686    -0.390058    -0.391179      13.87
 O       5.456820    -1.150885     0.313618     177.08
 C       5.495062    -1.131657     1.808325      99.89
 H       4.287237    -1.205612     1.975353      23.05
 H       5.826054    -0.128331     2.290258      25.90
 H       6.136110    -2.021029     2.185937      25.25
 C       4.543887    -0.653345    -1.756287      32.86
 O       5.494832    -1.290716    -2.456758     218.59
 H       6.115925    -1.911821    -1.966947      25.17
 C       3.596534     0.068576    -2.484444      50.92
 H       3.369347    -0.265130    -3.552509      22.49
 C       3.110969     1.585788    -0.667209      42.12
 C       2.370735     2.791523    -0.198250      87.94
 H       2.709459     3.593405    -1.102828      20.19
 O       2.653560     3.068710     1.303252     316.53
 H       3.617232     3.523908     1.308632      24.98
 C       0.687508     2.848181    -0.178054      49.67
 H       0.358677     2.513857    -1.164074      22.06
 C       0.065306     4.146758     0.376316      93.70
 O       0.599883     5.398515    -0.402533     232.61
 H       0.397983     5.133626    -1.341124      28.80
 H       0.401580     4.470248     1.437866      23.43
 H      -0.940950     4.057316     0.171098      25.23
 C      -0.944251    -1.411639    -0.672988      43.93
 H      -0.379563    -2.228068    -1.009158      19.91
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 C      -2.810382    -0.117070    -0.496367      64.35
 H      -3.905536     0.011953    -0.804584      18.76
 C      -2.089688     0.981957    -0.050938      22.50
 O      -2.656357     2.046035     0.734951     234.93
 C      -3.848577     2.504598     0.080227     115.28
 H      -3.696396     2.773523    -1.035538      25.96
 H      -4.653821     1.551382     0.085669      22.94
 H      -4.381588     3.472365     0.329218      25.71
 C      -0.680634     0.885706     0.274996       0.63
 O       0.135504     1.803884     0.740318     213.97
 C      -0.104931    -0.407776    -0.188999      23.32
 H       1.043575    -0.564804    -0.194910      19.10
 C      -2.328591    -1.298304    -0.881041      37.83
 C      -3.177426    -2.492221    -1.280890      68.05
 H      -4.261903    -2.303170    -1.773937      21.48
 O      -2.489119    -3.192330    -2.398958     226.45
 H      -2.539802    -4.253387    -2.411990      23.48
 C      -3.482705    -3.494539    -0.127690      97.45
 H      -2.572992    -3.983381     0.213137      26.07
 O      -3.948783    -2.829336     1.065664     329.14
 H      -3.254375    -2.465011     1.689123      26.02
 C      -4.764521    -4.306387    -0.592922      81.07
 O      -4.565044    -5.194917    -1.755588     317.75
 H      -5.144340    -5.022863    -2.480045      32.32
 H      -5.618998    -3.489242    -0.903543      25.35
 H      -5.217962    -4.916256     0.247511      26.23
55
name = lig-etoh-frame_161
 C       2.837240     1.242381    -2.025928      56.84
 H       2.048991     1.673094    -2.674572      21.14
 C       3.628545     0.650622     0.245553      50.04
 H       3.748234     1.058445     1.341090      22.86
 C       4.539818    -0.409201    -0.362961      30.34
 O       5.484456    -1.143503     0.288002     209.19
 C       5.488629    -1.086161     1.836279     117.18
 H       4.565576    -1.381287     2.144888      28.62
 H       5.684331    -0.190030     2.400413      28.13
 H       6.119339    -1.956605     2.170039      27.14
 C       4.577399    -0.630335    -1.736708      25.99
 O       5.524008    -1.310057    -2.425339     245.05
 H       6.103944    -1.868962    -2.023797      28.89
 C       3.548884     0.076975    -2.574030      43.76
 H       3.269802    -0.021278    -3.636194      25.22
 C       3.064533     1.589951    -0.626877      37.43
 C       2.330762     2.832219    -0.224379     104.67
 H       2.582709     3.482423    -0.955039      26.08
 O       2.676338     3.020731     1.244752     329.13
 H       3.402188     3.673471     1.519656      28.03
 C       0.827643     2.821047    -0.106911      61.79
 H       0.411664     2.686334    -1.162443      20.33
 C       0.126451     4.218010     0.322441      94.87
 O       0.642941     5.323835    -0.429928     287.44
 H       0.334043     5.176646    -1.325491      30.83
 H       0.262193     4.250715     1.378193      25.32
 H      -1.066482     4.152383     0.204448      22.66
 C      -0.949816    -1.450082    -0.748548      22.31
 H      -0.586040    -2.568209    -0.984664      19.14
 C      -2.783785    -0.064763    -0.437946      70.60
 H      -3.817616    -0.148878    -0.798230      21.14
 C      -2.004223     1.039627    -0.044622      28.76
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 O      -2.688582     2.007577     0.738807     206.59
 C      -3.960485     2.504501     0.048403     116.73
 H      -3.831985     2.768417    -1.040666      26.73
 H      -4.554180     1.735754     0.255121      27.08
 H      -4.021738     3.560736     0.415713      25.24
 C      -0.678963     0.828285     0.225224      15.09
 O       0.147211     1.792132     0.768773     224.15
 C      -0.147475    -0.289998    -0.199495      55.99
 H       0.863742    -0.581268     0.254664      18.83
 C      -2.313397    -1.275306    -0.825657      18.73
 C      -3.168522    -2.512129    -1.277365      78.07
 H      -4.013992    -2.033958    -1.723199      23.67
 O      -2.474965    -3.215259    -2.407218     219.53
 H      -2.583607    -4.276527    -2.507557      21.21
 C      -3.385836    -3.423423    -0.072545     102.15
 H      -2.401069    -3.960040     0.070839      24.52
 O      -3.989438    -2.845439     1.094007     294.92
 H      -3.227687    -2.304914     1.635936      23.00
 C      -4.747340    -4.232110    -0.549882      79.19
 O      -4.581925    -5.245739    -1.822711     225.68
 H      -5.113501    -4.829439    -2.657835      27.70
 H      -5.594601    -3.597541    -0.703781      27.50
 H      -5.020282    -4.867217     0.320111      27.26
55
name = lig-etoh-frame_162
 C       2.890591     1.207878    -2.057895      42.44
 H       1.961849     1.660669    -2.409654      18.32
 C       3.738864     0.691974     0.217852      34.89
 H       3.790532     0.733628     1.276497      21.34
 C       4.568670    -0.373957    -0.310325      14.36
 O       5.533693    -1.140131     0.327505     211.95
 C       5.469563    -1.071996     1.828550     110.43
 H       4.505088    -1.618342     2.384040      24.72
 H       5.725058    -0.060328     2.282745      26.40
 H       6.248946    -1.815155     2.082084      27.00
 C       4.538673    -0.556984    -1.765753       3.91
 O       5.554815    -1.336211    -2.430120     149.78
 H       6.083651    -1.955918    -1.684396      23.87
 C       3.498043     0.130458    -2.621538      58.87
 H       3.421683    -0.042508    -3.704137      29.14
 C       2.965300     1.550267    -0.638831      50.30
 C       2.305900     2.850682    -0.147091     122.54
 H       2.555872     3.873406    -0.827394      21.56
 O       2.691994     2.991626     1.193529     335.71
 H       3.304848     3.706631     1.339360      31.45
 C       0.867856     2.802299    -0.083999      84.25
 H       0.519681     2.732701    -1.085084      21.56
 C       0.174694     4.247750     0.265186     106.95
 O       0.687823     5.261037    -0.438388     274.20
 H       0.407931     5.237159    -1.502402      26.47
 H       0.264228     4.291416     1.409526      24.52
 H      -0.891529     4.156083     0.202157      25.32
 C      -0.887415    -1.476448    -0.792011      48.67
 H      -0.630507    -2.447717    -0.872064      25.71
 C      -2.814166    -0.000606    -0.423782      45.20
 H      -4.019709     0.145913    -0.514362      21.06
 C      -2.011219     1.093413     0.022177      16.22
 O      -2.722959     2.003749     0.704499     181.12
 C      -4.009698     2.544946     0.031704      84.22
 H      -3.889870     2.475397    -1.138372      24.41
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 H      -5.003827     1.894333     0.467994      22.73
 H      -3.917345     3.406271     0.720632      23.50
 C      -0.657763     0.850752     0.152878       9.62
 O       0.185224     1.806007     0.817773     218.23
 C      -0.154293    -0.362580    -0.236020      51.93
 H       0.718379    -0.443889     0.319946      18.77
 C      -2.249034    -1.317045    -0.807381      18.96
 C      -3.116260    -2.482098    -1.287019      73.41
 H      -4.066005    -1.891987    -1.657304      22.35
 O      -2.451320    -3.230650    -2.413879     243.42
 H      -2.831409    -4.057491    -2.323201      25.61
 C      -3.366526    -3.383275    -0.061477     107.06
 H      -2.507195    -4.055417     0.009236      22.84
 O      -4.003880    -2.838552     1.129929     316.73
 H      -3.324653    -2.341096     1.521565      29.30
 C      -4.687357    -4.229851    -0.525711      64.21
 O      -4.605233    -5.260168    -1.859416     230.75
 H      -4.931340    -4.693217    -2.560346      28.94
 H      -5.582487    -3.492065    -0.623000      25.74
 H      -4.776164    -5.010998     0.365075      26.20
55
name = lig-etoh-frame_163
 C       2.884096     1.198936    -2.022734      37.72
 H       2.052777     1.750038    -2.515055      18.48
 C       3.860607     0.719219     0.176272      60.22
 H       3.772396     0.671796     1.295305      19.99
 C       4.569133    -0.309103    -0.341793       4.84
 O       5.566866    -1.130589     0.405755     220.36
 C       5.452970    -1.101560     1.830751     126.05
 H       4.641341    -1.499172     2.251093      29.49
 H       5.656704    -0.033026     2.007402      26.77
 H       6.514529    -1.554762     2.057668      25.85
 C       4.492569    -0.480937    -1.815918      -0.19
 O       5.571376    -1.367894    -2.411780     174.07
 H       5.756718    -1.789321    -1.545094      25.75
 C       3.529475     0.145607    -2.641706      57.89
 H       3.645902    -0.190097    -3.716368      27.52
 C       2.902607     1.482138    -0.677481      65.57
 C       2.325532     2.864599    -0.072836     132.54
 H       2.521637     3.771933    -0.487921      23.58
 O       2.713959     2.978366     1.196244     295.85
 H       3.482133     3.694276     1.096560      25.64
 C       0.782279     2.818800    -0.091469      69.41
 H       0.508769     2.505576    -1.183672      18.11
 C       0.210630     4.181194     0.273556     101.93
 O       0.752807     5.264433    -0.480690     284.14
 H       0.667179     5.103274    -1.397023      32.19
 H       0.445412     4.594430     1.263538      24.10
 H      -0.941098     4.060272     0.050861      22.44
 C      -0.813419    -1.463841    -0.793535      54.18
 H      -0.285219    -2.541849    -0.840735      21.43
 C      -2.856994     0.010822    -0.448324      46.03
 H      -3.847035     0.324078    -0.234420      23.08
 C      -2.090170     1.072705     0.084894       6.03
 O      -2.771430     2.051392     0.664510     204.82
 C      -4.050877     2.543009     0.082732     117.91
 H      -4.008382     2.437314    -0.975218      27.73
 H      -4.969182     2.259812     0.375036      28.05
 H      -4.118904     3.524033     0.601796      25.74
 C      -0.621164     0.937926     0.088264       5.31
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 O       0.232431     1.816948     0.854027     209.03
 C      -0.124817    -0.488494    -0.268987      18.40
 H       1.012681    -0.451574     0.142936      15.29
 C      -2.221012    -1.295780    -0.820240      27.64
 C      -3.051717    -2.384877    -1.295878      83.45
 H      -4.088035    -2.106974    -1.574290      23.93
 O      -2.436262    -3.226884    -2.394243     168.02
 H      -3.161528    -4.048540    -2.206758      20.43
 C      -3.435531    -3.396641    -0.109271     104.91
 H      -2.630722    -4.118027     0.183192      22.56
 O      -3.999966    -2.828855     1.143096     290.64
 H      -3.231109    -2.271770     1.688500      22.14
 C      -4.602329    -4.299492    -0.509463      91.78
 O      -4.620496    -5.227014    -1.843509     250.75
 H      -4.835061    -4.609122    -2.550593      30.09
 H      -5.461840    -3.564203    -0.570860      27.07
 H      -4.723899    -5.034542     0.180229      29.01
55
name = lig-etoh-frame_164
 C       2.799408     1.220262    -2.011166      57.09
 H       2.326629     1.838889    -2.790121      19.24
 C       3.915152     0.762650     0.152516      77.27
 H       3.755774     0.946001     1.244045      16.74
 C       4.608528    -0.272680    -0.430426       6.18
 O       5.558253    -1.117199     0.426774     208.58
 C       5.524895    -1.085898     1.814946     119.21
 H       4.463027    -1.570622     2.275640      24.48
 H       5.426333     0.010018     2.084108      25.68
 H       6.410817    -1.446964     2.235046      27.83
 C       4.514658    -0.460043    -1.856810      24.64
 O       5.528935    -1.373298    -2.360403     215.80
 H       5.700514    -1.844069    -1.543433      27.20
 C       3.629950     0.125092    -2.653655      48.81
 H       3.660371    -0.139594    -3.671716      28.03
 C       2.908607     1.440782    -0.664943      83.51
 C       2.299112     2.793327    -0.051097     127.09
 H       2.683565     3.778685    -0.708355      21.03
 O       2.772117     2.995936     1.275130     318.24
 H       3.677848     3.397785     1.278390      30.44
 C       0.705223     2.825948    -0.122559      84.44
 H       0.426052     2.438985    -1.045200      19.19
 C       0.205089     4.125870     0.283879     103.48
 O       0.830268     5.291312    -0.532820     204.72
 H       0.920200     4.905397    -1.535480      26.28
 H       0.487756     4.571021     1.234199      24.40
 H      -0.877124     4.119700     0.073226      23.88
 C      -0.779186    -1.513565    -0.787673      32.50
 H      -0.288844    -2.393145    -1.000856      21.89
 C      -2.839063    -0.031846    -0.486986      49.41
 H      -4.013708     0.087741    -0.100322      20.69
 C      -2.110062     1.000514     0.115112     -10.21
 O      -2.834004     2.143513     0.648136     194.40
 C      -4.062110     2.580131     0.164382     108.84
 H      -4.107510     2.591671    -1.067991      24.26
 H      -5.111097     2.029107     0.528865      23.62
 H      -4.200420     3.727280     0.121498      24.33
 C      -0.613414     0.958234     0.050047       5.89
 O       0.264037     1.812733     0.855565     200.53
 C      -0.007392    -0.430307    -0.230522       6.73
 H       0.999427    -0.588080    -0.314884      17.87
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 C      -2.221676    -1.201114    -0.853595      32.04
 C      -3.024801    -2.344514    -1.289018      84.51
 H      -4.068954    -2.079904    -1.663074      23.23
 O      -2.456003    -3.223094    -2.339073     231.01
 H      -3.005542    -4.022262    -2.467459      25.23
 C      -3.483594    -3.438213    -0.137739      95.05
 H      -2.622588    -3.972762     0.277227      23.46
 O      -3.981958    -2.800601     1.141018     313.31
 H      -3.230737    -2.505214     1.680881      26.69
 C      -4.548273    -4.388120    -0.543300      98.30
 O      -4.618582    -5.155476    -1.788153     233.32
 H      -4.840688    -4.561365    -2.646856      28.50
 H      -5.488658    -3.775405    -0.550678      26.56
 H      -4.792485    -5.281984     0.290303      25.39
55
name = lig-etoh-frame_165
 C       2.745703     1.190663    -2.074564     136.02
 H       2.488904     1.951177    -2.843982      27.09
 C       3.902109     0.807897     0.126038      18.60
 H       3.927817     1.187080     1.131852      16.37
 C       4.674676    -0.240021    -0.462961       8.95
 O       5.536814    -1.104757     0.364532     233.17
 C       5.524708    -1.016755     1.831198     120.17
 H       4.761466    -1.614647     2.147679      28.31
 H       5.259009    -0.073450     2.341239      26.25
 H       6.402518    -1.537980     2.456224      25.39
 C       4.631022    -0.519498    -1.848019      25.35
 O       5.456866    -1.370815    -2.304550     212.86
 H       5.858253    -2.116908    -1.609966      22.16
 C       3.677149     0.173992    -2.650025      84.26
 H       3.576224     0.011483    -3.790305      20.06
 C       2.938590     1.458475    -0.624855      93.47
 C       2.286729     2.727697    -0.078389     109.03
 H       2.721909     3.309021    -0.813976      17.77
 O       2.813016     3.004211     1.376837     323.59
 H       3.779761     3.270971     1.437105      29.78
 C       0.725586     2.799307    -0.118165      69.35
 H       0.287227     2.547960    -1.186059      14.82
 C       0.187904     4.173490     0.264519      82.70
 O       0.894126     5.293503    -0.598883     222.88
 H       1.143023     4.828178    -1.504525      26.56
 H       0.421597     4.231255     1.399792      23.63
 H      -0.942610     4.277694     0.208465      22.77
 C      -0.788590    -1.460910    -0.747487      27.16
 H      -0.400277    -2.483668    -1.204792      18.43
 C      -2.853017    -0.056258    -0.474659      56.83
 H      -3.841136    -0.337610    -0.399294      21.90
 C      -2.087287     0.975118     0.123577     -12.22
 O      -2.850920     2.227887     0.647542     178.50
 C      -4.133840     2.635727     0.168266     120.65
 H      -4.180075     2.453384    -0.908695      27.20
 H      -4.708973     1.959069     0.673925      26.23
 H      -4.150474     3.693585     0.078224      26.10
 C      -0.618289     0.891929     0.080181      28.53
 O       0.255805     1.794234     0.822184     208.76
 C       0.062163    -0.318177    -0.222940      23.63
 H       1.171381    -0.501183    -0.611851      14.67
 C      -2.170581    -1.180420    -0.913793      18.60
 C      -3.092588    -2.397284    -1.279261      76.74
 H      -3.944830    -1.808100    -1.796610      22.88
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 O      -2.450817    -3.199827    -2.292312     264.63
 H      -2.866067    -4.013528    -2.556740      27.42
 C      -3.464419    -3.445554    -0.111512      94.22
 H      -2.459528    -3.871010     0.112349      24.99
 O      -3.981159    -2.779900     1.108595     324.43
 H      -3.123802    -2.670451     1.641988      24.83
 C      -4.585524    -4.503085    -0.555155     112.19
 O      -4.591680    -5.084982    -1.755114     320.58
 H      -4.909102    -4.577331    -2.472966      33.74
 H      -5.611884    -3.963944    -0.418428      27.17
 H      -4.600928    -5.177023     0.170023      29.17
55
name = lig-etoh-frame_166
 C       2.783318     1.130115    -2.120892      70.70
 H       2.345816     1.955683    -2.685531      23.86
 C       3.883410     0.822178     0.094115      61.50
 H       4.255405     1.279067     1.090617      23.50
 C       4.735495    -0.193620    -0.422274      27.00
 O       5.525947    -1.077457     0.287745     184.71
 C       5.509041    -0.962975     1.869941     105.05
 H       4.699551    -1.863243     2.116626      23.11
 H       5.281761    -0.026197     2.379101      24.68
 H       6.398922    -1.387241     2.185089      27.50
 C       4.679234    -0.521133    -1.775446      25.21
 O       5.451500    -1.453951    -2.305171     254.18
 H       5.810267    -2.109335    -1.736471      26.54
 C       3.681793     0.259420    -2.644247      60.67
 H       3.634327     0.133666    -3.682988      19.58
 C       2.945388     1.482593    -0.648933      66.18
 C       2.304843     2.655997    -0.071686     111.79
 H       2.775102     3.429797    -0.891448      15.78
 O       2.798319     2.984905     1.449172     273.65
 H       3.754220     3.469074     1.314709      25.73
 C       0.763141     2.773246    -0.132803      81.87
 H       0.442051     2.698699    -1.118883      17.22
 C       0.197136     4.259608     0.248243      93.51
 O       0.940562     5.264601    -0.629725     281.29
 H       1.112921     4.856394    -1.442136      33.48
 H       0.418874     4.172783     1.287494      24.71
 H      -0.943498     4.412905     0.224168      23.39
 C      -0.776674    -1.345074    -0.707601      49.39
 H      -0.502858    -2.291955    -1.169864      16.62
 C      -2.835772    -0.068128    -0.439971      44.31
 H      -3.988140    -0.425183    -0.699403      18.30
 C      -2.101555     1.010951     0.120694       0.57
 O      -2.781837     2.283307     0.649247     151.25
 C      -4.174500     2.658022     0.125308      86.49
 H      -4.367944     2.060339    -0.905094      23.34
 H      -4.844890     2.069527     0.944924      23.78
 H      -4.238395     3.782517     0.441910      23.47
 C      -0.619543     0.812967     0.179128       7.04
 O       0.210623     1.774268     0.765064     223.79
 C       0.076735    -0.283885    -0.302497      32.67
 H       1.112306    -0.099532    -0.452051      15.00
 C      -2.104033    -1.252756    -0.960015      23.26
 C      -3.176954    -2.444066    -1.283781      79.56
 H      -3.979385    -1.835779    -1.773811      24.21
 O      -2.411389    -3.160969    -2.266469     190.02
 H      -2.904081    -4.145426    -2.487164      21.87
 C      -3.444366    -3.418772    -0.093973      93.78
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 H      -2.445117    -3.908385    -0.071844      25.96
 O      -3.971144    -2.774779     1.057182     327.07
 H      -3.124983    -2.641887     1.710379      23.43
 C      -4.653508    -4.529069    -0.485871      91.22
 O      -4.543304    -5.065351    -1.784268     305.36
 H      -5.064278    -4.454529    -2.344504      31.58
 H      -5.603775    -4.060791    -0.241335      28.46
 H      -4.329130    -5.453435     0.318198      25.20
55
name = lig-etoh-frame_167
 C       2.833708     1.135998    -2.080326      72.37
 H       2.049552     1.722990    -2.620303      22.84
 C       3.915022     0.828638     0.097995     107.76
 H       4.279216     1.228410     0.965166      31.33
 C       4.766208    -0.154069    -0.389537      32.92
 O       5.533931    -1.035224     0.269858     195.45
 C       5.458797    -0.972804     1.865122     104.01
 H       4.775896    -1.713788     2.146641      25.96
 H       5.289151     0.075200     2.216313      24.76
 H       6.614569    -1.203982     1.907523      24.07
 C       4.639276    -0.452134    -1.724754      17.76
 O       5.472796    -1.565556    -2.360528     216.04
 H       5.740398    -2.169109    -1.624765      25.87
 C       3.742557     0.285188    -2.620414      35.73
 H       3.821503     0.110063    -3.742246      19.52
 C       2.951347     1.461085    -0.721874      51.72
 C       2.342793     2.670509    -0.046897     121.48
 H       2.579780     3.639745    -0.432045      17.54
 O       2.761563     2.953655     1.456780     319.34
 H       3.408335     3.656275     1.326580      29.56
 C       0.788886     2.785802    -0.139105      45.52
 H       0.568309     2.583403    -1.285674      15.43
 C       0.245141     4.316643     0.209674      93.60
 O       0.969229     5.231603    -0.604214     238.37
 H       0.912288     4.803896    -1.662104      23.95
 H       0.602428     4.594304     1.307398      22.19
 H      -0.829343     4.413499     0.043879      23.50
 C      -0.730995    -1.281150    -0.723888      52.69
 H      -0.199631    -2.228437    -1.045999      17.51
 C      -2.818836    -0.114787    -0.440990      44.04
 H      -3.817855     0.130767    -0.631089      20.92
 C      -2.145897     1.060752     0.118680     -11.70
 O      -2.679511     2.307692     0.625935     157.26
 C      -4.200364     2.609036     0.146141     118.75
 H      -4.505772     2.190101    -0.732096      27.91
 H      -4.947323     2.406692     0.865666      27.52
 H      -4.335997     3.629866     0.394268      26.49
 C      -0.657466     0.784495     0.288795       0.68
 O       0.154346     1.774466     0.712115     204.07
 C       0.037387    -0.250124    -0.386506      40.87
 H       1.132388     0.006672    -0.243155      13.28
 C      -2.143579    -1.285862    -0.930636      29.04
 C      -3.179658    -2.447564    -1.297609      82.74
 H      -4.233671    -2.076164    -1.694667      23.37
 O      -2.378011    -3.159499    -2.272531     253.52
 H      -2.812657    -3.958939    -2.287161      27.72
 C      -3.470477    -3.404144    -0.121471      99.00
 H      -2.567658    -4.024857     0.020536      23.46
 O      -3.940014    -2.773981     1.027285     353.27
 H      -3.323835    -2.431708     1.637543      29.43
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 C      -4.634961    -4.552344    -0.335130      88.69
 O      -4.501740    -5.052762    -1.842063     276.38
 H      -5.246040    -4.422141    -2.251533      28.86
 H      -5.717419    -4.146545    -0.044903      27.22
 H      -4.377046    -5.375486     0.123205      28.76
55
name = lig-etoh-frame_168
 C       2.844519     1.193459    -2.035473     110.02
 H       1.973754     1.364110    -2.652924      22.31
 C       3.961329     0.846368     0.102383      60.19
 H       4.068591     1.340266     1.169287      21.58
 C       4.758605    -0.138510    -0.390465      21.56
 O       5.555648    -0.999521     0.316771     243.34
 C       5.473130    -0.964185     1.784944     116.76
 H       4.701537    -1.729881     2.310872      24.70
 H       5.222681     0.044681     2.051156      25.81
 H       6.505364    -1.114906     2.041602      26.76
 C       4.618299    -0.426756    -1.782219      16.50
 O       5.468791    -1.633914    -2.403998     158.97
 H       5.586823    -2.186932    -1.463577      22.97
 C       3.851079     0.252106    -2.612618      63.71
 H       3.958356     0.018210    -3.659073      24.04
 C       2.990120     1.456619    -0.728499      56.04
 C       2.342043     2.741366     0.026018     141.20
 H       2.611740     3.819125    -0.298679      18.82
 O       2.700898     2.896019     1.421762     289.79
 H       3.194077     3.831711     1.508115      27.69
 C       0.796385     2.807591    -0.156260      57.90
 H       0.613095     2.504716    -1.144601      23.56
 C       0.333202     4.333099     0.196932     109.29
 O       0.999672     5.199779    -0.622807     289.00
 H       0.745472     5.059221    -1.488241      32.44
 H       0.531148     4.844214     1.082106      24.44
 H      -0.816164     4.309130    -0.093281      23.23
 C      -0.710381    -1.344777    -0.817899      19.40
 H       0.071355    -2.173472    -0.886902      15.80
 C      -2.800949    -0.089224    -0.438922      46.52
 H      -3.819922     0.471752    -0.581956      18.82
 C      -2.132496     1.057345     0.129039       9.93
 O      -2.617580     2.302829     0.568571     142.80
 C      -4.182392     2.568328     0.236188      95.23
 H      -4.570256     2.346748    -0.939575      23.67
 H      -4.983543     2.230328     1.001372      24.84
 H      -4.181986     3.743391    -0.019177      24.30
 C      -0.751477     0.828081     0.323418      17.04
 O       0.113887     1.820246     0.697155     223.53
 C      -0.020052    -0.148411    -0.403624      32.96
 H       1.090669    -0.336568    -0.171093      15.69
 C      -2.241841    -1.278913    -0.847701      31.96
 C      -3.127177    -2.433564    -1.313500      87.54
 H      -4.175128    -2.195776    -1.643902      24.19
 O      -2.351576    -3.160850    -2.291740     208.55
 H      -2.804789    -4.125189    -2.281348      21.39
 C      -3.510603    -3.441875    -0.141614     106.27
 H      -2.641768    -4.050858     0.186061      22.89
 O      -3.941137    -2.763039     1.018667     318.47
 H      -3.182911    -2.150041     1.530609      21.57
 C      -4.587255    -4.534097    -0.252791      89.27
 O      -4.492002    -5.016984    -1.864844     288.52
 H      -5.226535    -4.606277    -2.285846      32.25
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 H      -5.567407    -4.282350    -0.020130      28.01
 H      -4.355044    -5.619021     0.312262      24.44
55
name = lig-etoh-frame_169
 C       2.886122     1.196117    -2.062856      82.40
 H       2.009632     1.284002    -2.708216      21.96
 C       4.001381     0.903165     0.141157      58.79
 H       3.824181     1.216784     1.112717      21.35
 C       4.739172    -0.158521    -0.412078      19.41
 O       5.584658    -0.984538     0.374507     260.14
 C       5.485395    -0.946179     1.705429     131.83
 H       4.811856    -1.627891     2.258627      27.55
 H       5.115399     0.066106     2.044633      26.53
 H       6.453481    -1.179664     2.344627      25.92
 C       4.699903    -0.506119    -1.841558      15.30
 O       5.429309    -1.646903    -2.395203     260.80
 H       5.516746    -2.201982    -1.675675      29.41
 C       3.883007     0.266819    -2.631053      61.31
 H       3.919776    -0.060353    -3.685440      25.18
 C       3.034019     1.536843    -0.643881      63.30
 C       2.316929     2.826172     0.077799     131.53
 H       2.800709     3.606059    -0.587333      20.53
 O       2.632833     2.837816     1.402960     337.88
 H       3.112449     3.636710     1.649265      30.01
 C       0.806750     2.832021    -0.129869      72.72
 H       0.516100     2.596511    -1.228626      20.94
 C       0.362505     4.290633     0.163242     103.78
 O       1.053240     5.220069    -0.663336     275.74
 H       0.687828     5.192240    -1.663368      26.42
 H       0.356277     4.719721     1.288531      23.72
 H      -0.677554     4.278612    -0.002243      25.17
 C      -0.737114    -1.374948    -0.894576      21.15
 H      -0.285959    -2.290468    -1.057427      22.43
 C      -2.833253     0.034644    -0.421001      58.35
 H      -3.883132     0.085151    -0.674996      24.15
 C      -2.092068     1.020911     0.153121      23.89
 O      -2.620928     2.282921     0.488734     193.86
 C      -4.139655     2.577249     0.275006     122.18
 H      -4.360211     2.214901    -0.647925      29.14
 H      -4.664033     2.063328     1.055003      26.62
 H      -3.983916     3.554501    -0.009399      26.91
 C      -0.781902     0.927214     0.262883      18.43
 O       0.085844     1.909232     0.737431     230.60
 C      -0.117723    -0.137762    -0.385130      35.32
 H       0.882815    -0.338898    -0.249859      18.18
 C      -2.277685    -1.287783    -0.773529       9.80
 C      -3.068017    -2.455695    -1.315052      75.40
 H      -4.058375    -2.017463    -1.788195      22.38
 O      -2.335531    -3.176887    -2.315933     204.67
 H      -2.737245    -4.157535    -2.416150      21.38
 C      -3.510668    -3.498861    -0.107376      98.26
 H      -2.542479    -3.966236     0.155170      22.67
 O      -3.961250    -2.716857     1.037262     333.55
 H      -3.126790    -2.295066     1.246318      25.56
 C      -4.517522    -4.570412    -0.259125      86.04
 O      -4.484990    -4.984403    -1.833518     284.79
 H      -5.271887    -4.716086    -2.347140      31.17
 H      -5.645805    -4.214464    -0.047094      25.81
 H      -4.314286    -5.396814     0.367730      26.75
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name = lig-etoh-frame_170
 C       2.971544     1.166400    -2.075474      45.33
 H       2.127613     1.537748    -2.697114      22.30
 C       4.021739     0.944572     0.149989      48.22
 H       3.881210     1.016630     1.296902      19.90
 C       4.737201    -0.204772    -0.441192      22.09
 O       5.624611    -0.988496     0.371152     234.97
 C       5.500224    -0.893209     1.738538     124.79
 H       4.655917    -1.751700     2.072939      25.01
 H       5.142277     0.038535     2.103799      26.66
 H       6.369737    -1.170922     2.334934      27.49
 C       4.809306    -0.596385    -1.840099      16.04
 O       5.374482    -1.619428    -2.382309     234.65
 H       5.542224    -2.416156    -1.747955      24.15
 C       3.865275     0.294150    -2.662694      43.51
 H       3.684380    -0.028355    -3.727684      23.16
 C       3.055563     1.642192    -0.600081      49.84
 C       2.310848     2.835488     0.027183     125.80
 H       2.817790     3.531325    -0.636739      19.97
 O       2.566845     2.787875     1.432503     323.81
 H       3.241222     3.465266     1.650869      27.54
 C       0.805129     2.869355    -0.120129      97.81
 H       0.517774     2.762500    -1.144659      19.87
 C       0.349417     4.256702     0.154566      96.77
 O       1.104870     5.274030    -0.698354     238.61
 H       0.835211     5.061484    -1.698118      26.56
 H       0.437308     4.305848     1.192599      25.96
 H      -0.837974     4.338663    -0.026618      22.94
 C      -0.872234    -1.327880    -0.909414      49.46
 H      -0.682898    -2.414091    -1.379467      19.98
 C      -2.897386     0.044026    -0.435058      65.01
 H      -3.965334    -0.180490    -0.637386      23.16
 C      -2.141810     1.054849     0.181248      14.17
 O      -2.648846     2.269621     0.413066     201.40
 C      -4.012967     2.555030     0.295829     103.27
 H      -4.358028     1.770759    -0.614833      23.00
 H      -4.517588     2.143975     1.236052      25.66
 H      -4.059761     3.766515     0.357234      23.56
 C      -0.674536     1.011145     0.151080      18.25
 O       0.057894     2.012140     0.807835     215.52
 C      -0.219973    -0.227310    -0.365564      35.52
 H       1.004139    -0.044158    -0.353166      16.70
 C      -2.225559    -1.269136    -0.731176      17.14
 C      -3.060836    -2.493229    -1.307516      72.64
 H      -3.887904    -1.942507    -1.846540      23.46
 O      -2.312113    -3.201355    -2.344194     255.68
 H      -2.736089    -3.975460    -2.467522      28.20
 C      -3.465704    -3.508585    -0.057168      90.46
 H      -2.446316    -3.912461     0.102178      23.32
 O      -3.990243    -2.680106     1.033593     323.49
 H      -3.109685    -2.326114     1.404210      23.70
 C      -4.513736    -4.593289    -0.357821      99.10
 O      -4.465154    -4.964664    -1.760528     297.05
 H      -5.388497    -4.793569    -2.239492      29.52
 H      -5.407181    -4.155429    -0.129575      28.86
 H      -4.207232    -5.486882     0.401206      24.80
55
name = lig-etoh-frame_171
 C       3.045092     1.192963    -2.030189      57.96
 H       2.411601     1.855899    -2.636268      24.36
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 C       4.021909     0.938984     0.140814      44.94
 H       4.160240     0.871687     1.201709      22.24
 C       4.762492    -0.245029    -0.461715      25.81
 O       5.676603    -0.989409     0.328874     200.71
 C       5.463011    -0.886096     1.834945     114.56
 H       4.676093    -1.591895     1.864535      27.52
 H       5.182919     0.141422     2.203929      25.32
 H       6.493870    -1.191896     2.221549      26.95
 C       4.802823    -0.548962    -1.792805      21.43
 O       5.352413    -1.638155    -2.393375     210.79
 H       5.580812    -2.547490    -1.872643      23.36
 C       3.867603     0.255675    -2.671601      45.03
 H       3.537150     0.058088    -3.669247      22.18
 C       3.096744     1.675216    -0.631020      38.73
 C       2.323301     2.777684    -0.052855     109.07
 H       2.689361     3.896370    -0.381854      17.51
 O       2.513246     2.770123     1.477179     259.73
 H       3.478486     3.228543     1.536208      25.02
 C       0.796586     2.912787    -0.148305      80.63
 H       0.516990     2.613647    -1.212469      19.21
 C       0.296411     4.274521     0.127877     101.38
 O       1.134629     5.315514    -0.694768     214.13
 H       1.048872     4.925678    -1.639304      27.93
 H       0.685901     4.318381     1.259213      23.27
 H      -0.684159     4.399189    -0.083513      26.28
 C      -0.999120    -1.308299    -0.905817      68.68
 H      -0.611267    -2.068453    -1.491379      24.87
 C      -2.944268    -0.056158    -0.446756      59.57
 H      -4.088969    -0.068229    -0.363096      23.33
 C      -2.187239     1.091947     0.161339      -8.20
 O      -2.645173     2.301533     0.362006     220.07
 C      -3.925888     2.509367     0.322347     154.52
 H      -4.486657     2.028326    -0.357851      29.79
 H      -4.425089     2.307329     1.291392      27.30
 H      -4.291281     3.474911     0.464222      28.15
 C      -0.627884     1.034027     0.048646      -9.42
 O       0.034311     2.096173     0.856469     176.27
 C      -0.181455    -0.264073    -0.339042      46.88
 H       0.784753    -0.146090    -0.537221      22.29
 C      -2.254859    -1.226331    -0.728882      33.42
 C      -3.065166    -2.511057    -1.276800      70.66
 H      -3.965006    -2.004070    -1.843837      23.15
 O      -2.275067    -3.207627    -2.356645     182.50
 H      -2.940398    -4.068965    -2.565226      21.27
 C      -3.402589    -3.464638    -0.042232      92.38
 H      -2.444092    -3.950510     0.250152      24.01
 O      -4.000237    -2.659428     1.010056     293.13
 H      -3.388128    -2.357891     1.852287      22.94
 C      -4.483010    -4.608937    -0.437179      96.59
 O      -4.449832    -4.962855    -1.704220     336.94
 H      -5.334238    -4.891288    -1.987971      31.27
 H      -5.493075    -4.066546    -0.099947      27.23
 H      -4.311818    -5.527861     0.186385      25.97
55
name = lig-etoh-frame_172
 C       3.109327     1.286311    -1.980150      90.17
 H       2.667522     2.015067    -2.666537      25.61
 C       4.045568     0.856805     0.095693      54.77
 H       4.256679     1.062972     1.144449      22.86
 C       4.797086    -0.229646    -0.422785      29.40
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 O       5.723956    -0.973179     0.299881     176.56
 C       5.446107    -0.884049     1.888027     100.19
 H       4.559648    -1.589965     2.110856      26.52
 H       5.314268     0.116473     2.256957      25.98
 H       6.479116    -1.294058     2.162808      26.80
 C       4.712139    -0.478225    -1.806002      24.73
 O       5.354940    -1.681317    -2.427962     216.37
 H       5.503346    -2.369946    -1.873867      27.69
 C       3.870009     0.204687    -2.614346      54.91
 H       3.626101     0.006321    -3.714052      21.50
 C       3.177856     1.632174    -0.692163      38.61
 C       2.329332     2.779246    -0.065553     130.02
 H       2.561711     3.797347    -0.161092      19.26
 O       2.498792     2.770978     1.488654     306.48
 H       3.406770     2.971184     1.529909      29.81
 C       0.779443     2.914111    -0.222712      75.24
 H       0.481527     2.416534    -1.149967      18.86
 C       0.326228     4.348922     0.118397      95.63
 O       1.133360     5.338036    -0.659027     215.96
 H       1.291556     4.914382    -1.648617      25.08
 H       0.612295     4.693125     1.061173      24.62
 H      -0.855846     4.515675    -0.098961      22.80
 C      -0.960642    -1.256405    -0.879970      21.39
 H      -0.325189    -1.945280    -1.508240      23.88
 C      -3.000950    -0.079906    -0.378621      65.23
 H      -4.002387     0.049830    -0.152639      26.00
 C      -2.149707     1.044109     0.055104       1.07
 O      -2.575046     2.369821     0.322357     175.57
 C      -3.989486     2.488722     0.415243     113.07
 H      -4.769330     2.148773    -0.496877      24.35
 H      -4.329232     2.086010     1.406992      26.14
 H      -4.273184     3.643213     0.234144      24.68
 C      -0.703411     1.018998     0.022295       1.19
 O       0.011597     2.137063     0.843173     120.65
 C      -0.113913    -0.242683    -0.334487      27.81
 H       1.046143    -0.535694    -0.736995      20.71
 C      -2.440828    -1.247219    -0.777359      28.51
 C      -3.069686    -2.498547    -1.247742      86.58
 H      -4.081669    -2.256802    -1.673725      23.35
 O      -2.261137    -3.221683    -2.346159     223.84
 H      -2.897400    -3.924751    -2.650083      23.85
 C      -3.342984    -3.421007    -0.038915     107.74
 H      -2.495191    -3.929891     0.420975      24.55
 O      -4.021024    -2.643726     1.000348     310.09
 H      -3.545982    -2.546496     1.773446      30.75
 C      -4.453738    -4.551045    -0.382620     103.71
 O      -4.435116    -4.985742    -1.735185     322.52
 H      -5.354407    -5.026801    -2.021312      31.72
 H      -5.399850    -4.187251    -0.154699      29.32
 H      -4.379053    -5.580721     0.226086      25.04
55
name = lig-etoh-frame_173
 C       3.181524     1.380517    -2.041430      44.90
 H       2.715875     2.061829    -2.744741      20.99
 C       4.086920     0.759867     0.087252      76.86
 H       4.188571     1.365672     1.041886      23.69
 C       4.838435    -0.193441    -0.384467      29.91
 O       5.746683    -0.950108     0.319992     177.75
 C       5.462779    -0.923343     1.875503     105.20
 H       4.594714    -1.440783     2.430309      25.73
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 H       5.440936     0.127205     2.211226      25.46
 H       6.321450    -1.404692     2.289642      28.26
 C       4.658038    -0.526586    -1.840741      17.70
 O       5.345269    -1.671889    -2.466062     181.01
 H       5.437029    -2.314048    -1.613917      24.21
 C       3.813088     0.219893    -2.566401      61.91
 H       3.883254    -0.085418    -3.575127      27.14
 C       3.244883     1.601780    -0.690742      54.00
 C       2.323167     2.774828    -0.000136     121.84
 H       2.840729     3.862030    -0.357159      20.81
 O       2.488654     2.760939     1.461560     299.46
 H       3.456135     2.948688     1.664022      27.60
 C       0.755820     2.884769    -0.256228      73.60
 H       0.415406     2.525469    -1.239903      22.53
 C       0.352079     4.456944     0.055787     106.96
 O       1.133124     5.354419    -0.630038     308.81
 H       1.211091     5.146809    -1.515332      33.84
 H       0.444825     4.867393     1.156913      24.82
 H      -0.663743     4.524159    -0.044532      26.99
 C      -0.913151    -1.186924    -0.844190       7.97
 H      -0.343488    -2.040780    -1.326221      20.63
 C      -3.042354    -0.029841    -0.268463      40.90
 H      -4.193361     0.123834    -0.005012      18.31
 C      -2.085487     1.005981    -0.078293      18.67
 O      -2.517271     2.414456     0.271893     107.54
 C      -4.135684     2.523475     0.487609     114.08
 H      -4.539060     2.082525    -0.333502      27.52
 H      -4.303576     1.936006     1.396983      25.34
 H      -4.016702     3.546349     0.325603      26.36
 C      -0.765146     0.987949     0.074534       7.98
 O      -0.025638     2.126576     0.764334     151.90
 C      -0.037269    -0.218027    -0.384733      45.73
 H       0.907374    -0.476806    -0.514281      22.89
 C      -2.515774    -1.281280    -0.862694       7.54
 C      -3.093827    -2.514886    -1.246767      89.40
 H      -4.230542    -2.560815    -1.536945      22.65
 O      -2.260756    -3.211251    -2.310230     253.78
 H      -2.845244    -3.868189    -2.667123      25.77
 C      -3.325306    -3.422098    -0.009788     107.10
 H      -2.398178    -3.843860     0.450376      25.80
 O      -4.070017    -2.634574     0.971502     280.03
 H      -3.299507    -2.607583     1.743943      23.35
 C      -4.405061    -4.501386    -0.292973      81.76
 O      -4.415151    -5.012789    -1.801574     256.49
 H      -5.384093    -5.213055    -2.178448      30.26
 H      -5.488493    -4.078653    -0.127189      26.53
 H      -4.296299    -5.403408     0.415231      25.51
55
name = lig-etoh-frame_174
 C       3.243229     1.465779    -2.143033      34.12
 H       2.594430     2.079999    -2.764340      18.76
 C       4.070061     0.785988     0.137382      60.98
 H       4.225627     1.208333     1.082960      25.14
 C       4.909635    -0.233606    -0.434717      17.39
 O       5.754052    -0.948364     0.397091     216.07
 C       5.507154    -0.950089     1.844687     111.16
 H       4.543196    -1.333276     2.272276      26.00
 H       5.613916     0.126786     2.090343      25.72
 H       6.332181    -1.577244     2.441775      25.58
 C       4.656265    -0.636840    -1.808342      19.83
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 O       5.316780    -1.634456    -2.464544     200.67
 H       5.482160    -2.259594    -1.645698      23.84
 C       3.757077     0.259605    -2.562856      48.67
 H       3.926653    -0.054901    -3.648845      26.62
 C       3.257735     1.600985    -0.668045      27.31
 C       2.366856     2.777854     0.052032     117.29
 H       2.841855     3.534567    -0.487665      25.28
 O       2.487330     2.744181     1.419695     309.82
 H       3.388800     3.154240     1.760888      27.19
 C       0.742802     2.883232    -0.238682      64.94
 H       0.480595     2.841744    -1.344015      21.56
 C       0.373333     4.520915     0.032792      97.02
 O       1.157383     5.414523    -0.603144     250.22
 H       0.951215     5.315326    -1.715135      23.41
 H       0.379277     4.581747     1.113028      26.26
 H      -0.813350     4.549678    -0.265213      23.35
 C      -0.935876    -1.183309    -0.836320      33.42
 H      -0.560087    -2.152539    -1.094663      20.00
 C      -3.069631    -0.032572    -0.201408      43.49
 H      -4.049123     0.111027    -0.024631      20.72
 C      -2.115982     1.065445    -0.157314      -9.78
 O      -2.507084     2.410928     0.215131      54.86
 C      -4.178780     2.549853     0.542329      84.36
 H      -4.536229     1.909832    -0.396138      22.35
 H      -4.444910     2.044256     1.496372      25.95
 H      -4.133972     3.700835     0.713269      24.17
 C      -0.684682     0.943057     0.145998       8.64
 O      -0.079074     2.076103     0.641003     200.98
 C      -0.053259    -0.154365    -0.420336      36.65
 H       1.199528    -0.222621    -0.245635      18.63
 C      -2.451309    -1.183592    -0.902123      -1.86
 C      -3.154738    -2.601900    -1.269754      84.68
 H      -4.161089    -2.485066    -1.652445      23.95
 O      -2.269675    -3.178266    -2.252898     216.17
 H      -2.883923    -4.011398    -2.688602      20.30
 C      -3.334449    -3.451120     0.022011     110.40
 H      -2.341539    -3.743558     0.355058      26.90
 O      -4.089071    -2.634926     0.971616     311.43
 H      -3.346875    -2.265534     1.548624      25.19
 C      -4.390723    -4.480360    -0.248289      76.68
 O      -4.386718    -5.036263    -1.843105     281.63
 H      -5.255446    -5.297546    -2.109131      33.95
 H      -5.306959    -3.940033    -0.124798      28.22
 H      -4.199269    -5.284163     0.525008      25.19
55
name = lig-etoh-frame_175
 C       3.276672     1.526817    -2.168950      28.22
 H       2.498321     2.074020    -2.730494      19.77
 C       4.055595     0.838204     0.157647      43.55
 H       4.245926     0.866557     1.306931      22.70
 C       4.937818    -0.277817    -0.478428       9.16
 O       5.774357    -0.985191     0.471524     216.70
 C       5.573221    -0.961175     1.832300     121.91
 H       4.414045    -1.194836     1.834365      24.43
 H       5.775450     0.055268     2.180707      27.05
 H       6.245940    -1.592835     2.264980      28.64
 C       4.626714    -0.670328    -1.746262      30.78
 O       5.292308    -1.613422    -2.445338     231.36
 H       5.625457    -2.315041    -1.948559      27.58
 C       3.778675     0.253330    -2.602691      37.91
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 H       3.684972     0.123478    -3.673539      26.53
 C       3.226466     1.621521    -0.665196      25.43
 C       2.394675     2.722404     0.033413     112.90
 H       2.807955     3.728720    -0.604127      22.37
 O       2.509142     2.742907     1.415076     337.01
 H       3.165952     3.374491     1.617828      29.62
 C       0.769609     2.941137    -0.231907      69.56
 H       0.627571     2.874661    -1.287255      23.55
 C       0.315299     4.480119     0.038022     104.69
 O       1.199050     5.508309    -0.619664     233.27
 H       0.831796     5.442477    -1.481856      30.07
 H       0.415841     4.483278     1.152735      25.57
 H      -0.588630     4.615964    -0.432606      26.50
 C      -0.998991    -1.213851    -0.854914      46.24
 H      -0.646699    -2.339105    -0.916444      19.43
 C      -3.008653    -0.047115    -0.211911      49.02
 H      -4.191735     0.047811    -0.068860      20.01
 C      -2.184544     1.162704    -0.140245     -14.43
 O      -2.558555     2.388829     0.168069     111.62
 C      -4.131107     2.570323     0.576690     108.29
 H      -4.730613     2.230240    -0.231795      26.56
 H      -4.483165     2.131216     1.528126      26.80
 H      -4.500729     3.549011     0.856611      27.24
 C      -0.635657     0.920847     0.155981       8.32
 O      -0.112119     2.039605     0.519129     198.72
 C      -0.048538    -0.120482    -0.429070      54.83
 H       0.936540    -0.054515    -0.119391      22.36
 C      -2.342723    -1.072453    -0.886635      14.18
 C      -3.182629    -2.630777    -1.277534      73.52
 H      -4.111735    -2.187240    -1.884307      22.90
 O      -2.299160    -3.175785    -2.207698     272.14
 H      -2.684209    -3.945365    -2.517188      27.56
 C      -3.355018    -3.449796     0.012679     105.21
 H      -2.338249    -3.773789     0.360112      25.61
 O      -4.086570    -2.626976     0.985799     281.98
 H      -3.488442    -1.984575     1.490126      24.79
 C      -4.381722    -4.505092    -0.266200      77.85
 O      -4.335370    -5.046390    -1.824536     275.11
 H      -5.242491    -5.349803    -1.961794      32.67
 H      -5.320431    -3.909789    -0.148656      27.19
 H      -4.286502    -5.422520     0.541982      24.65
55
name = lig-etoh-frame_176
 C       3.286815     1.507704    -2.108896      18.50
 H       2.583355     2.064886    -2.720104      21.19
 C       4.090381     0.834209     0.140804      55.34
 H       3.979311     0.727162     1.190360      24.83
 C       4.902379    -0.259858    -0.399454       5.36
 O       5.818812    -1.034791     0.446884     200.80
 C       5.575943    -0.934552     1.820718     115.03
 H       4.536452    -1.112316     1.913140      27.04
 H       5.896755    -0.029317     2.433705      26.48
 H       6.225063    -1.899162     2.230489      24.94
 C       4.579118    -0.644539    -1.736365      17.61
 O       5.272897    -1.611560    -2.453085     169.72
 H       5.797223    -2.500770    -2.123361      21.22
 C       3.827277     0.272916    -2.627444      47.16
 H       3.529722     0.076073    -3.682592      25.08
 C       3.197737     1.649671    -0.667852      41.81
 C       2.378975     2.712320    -0.059400     133.85
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 H       2.662615     3.698229    -0.324817      25.33
 O       2.550176     2.755265     1.431124     286.70
 H       3.093528     3.633917     1.509388      26.63
 C       0.836606     2.999782    -0.264817      65.04
 H       0.702004     2.662935    -1.363834      22.88
 C       0.305950     4.403498     0.055569      86.37
 O       1.227494     5.586533    -0.595897     149.28
 H       0.918047     5.575505    -1.600677      25.70
 H       0.309957     4.712321     1.164639      24.51
 H      -0.720689     4.629982    -0.433427      23.93
 C      -0.958972    -1.257589    -0.862512      47.60
 H      -0.615321    -2.197512    -0.940300      22.47
 C      -2.955875     0.021180    -0.259505      69.00
 H      -3.989162    -0.118919    -0.244066      21.83
 C      -2.224133     1.163204    -0.058438      12.18
 O      -2.685518     2.418871     0.149984     193.03
 C      -4.067621     2.589322     0.618240     115.27
 H      -4.908058     2.429340    -0.207562      25.05
 H      -4.242378     1.891006     1.482755      26.11
 H      -4.451126     3.653582     0.751578      25.61
 C      -0.740703     0.946299     0.072475      10.70
 O      -0.090801     2.082365     0.445543     174.56
 C      -0.085884    -0.177603    -0.433169      33.41
 H       1.109168    -0.277613    -0.185959      20.94
 C      -2.297872    -1.063736    -0.848848      21.70
 C      -3.176275    -2.525317    -1.283138      88.91
 H      -4.024020    -2.158709    -1.746626      27.16
 O      -2.306159    -3.186719    -2.175068     239.92
 H      -2.645493    -4.119029    -2.437555      23.69
 C      -3.382212    -3.409373    -0.012651     103.19
 H      -2.464195    -3.832039     0.381331      27.35
 O      -4.093875    -2.626343     0.998280     263.79
 H      -3.423882    -1.886784     1.454769      23.69
 C      -4.393558    -4.577455    -0.322499      99.50
 O      -4.276926    -5.043160    -1.743844     279.28
 H      -5.256032    -5.427083    -1.850910      29.70
 H      -5.424753    -4.107423    -0.227305      27.18
 H      -4.425502    -5.451456     0.302303      26.71
55
name = lig-etoh-frame_177
 C       3.272676     1.427569    -2.020996      55.70
 H       2.762855     2.097659    -2.733267      23.90
 C       4.105338     0.804011     0.107689      64.32
 H       3.751189     0.910066     1.180483      23.66
 C       4.839393    -0.228294    -0.304870      14.49
 O       5.848966    -1.056810     0.355774     191.58
 C       5.596079    -0.959858     1.852862     117.43
 H       4.481656    -1.072696     2.321547      26.37
 H       6.039883    -0.151861     2.391289      28.57
 H       5.931494    -1.842571     2.189762      29.83
 C       4.569412    -0.600849    -1.763328      10.76
 O       5.258978    -1.625853    -2.490078     187.94
 H       5.629641    -2.373905    -1.939060      24.96
 C       3.874470     0.312257    -2.611386      57.65
 H       3.610540    -0.125623    -3.594805      24.36
 C       3.217573     1.645725    -0.684591      41.62
 C       2.326466     2.752306    -0.089691     111.93
 H       2.815982     3.873861    -0.279699      19.47
 O       2.605619     2.783708     1.434748     279.34
 H       3.079310     3.681154     1.541198      25.46
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 C       0.892186     2.982391    -0.358337      85.16
 H       0.706007     2.742413    -1.369820      23.70
 C       0.325705     4.398114     0.040111      90.27
 O       1.219598     5.626875    -0.552532     151.25
 H       1.250063     5.597688    -1.611757      26.26
 H       0.238831     4.740130     1.024133      25.70
 H      -0.738935     4.440168    -0.227459      24.98
 C      -0.854002    -1.272444    -0.850491      26.92
 H      -0.375038    -2.332458    -1.187232      25.47
 C      -2.930590     0.064944    -0.353150      61.27
 H      -4.057116    -0.062030    -0.370119      25.89
 C      -2.211877     1.144404     0.050999      26.70
 O      -2.823431     2.485317     0.139388     201.42
 C      -4.052035     2.600442     0.639998     127.23
 H      -4.800015     2.342020    -0.107696      27.09
 H      -4.061810     1.827332     1.399667      26.40
 H      -3.921093     3.701616     0.877065      24.87
 C      -0.865389     1.022373    -0.067268       0.79
 O      -0.050086     2.156801     0.418297     137.57
 C      -0.125466    -0.260736    -0.404928      43.42
 H       0.937305    -0.547454    -0.495490      24.27
 C      -2.317296    -1.158543    -0.812089       9.06
 C      -3.109160    -2.365564    -1.246383      80.06
 H      -4.255999    -2.156666    -1.641842      22.93
 O      -2.293109    -3.203783    -2.170849     174.35
 H      -2.751454    -4.205207    -2.212220      18.90
 C      -3.446213    -3.366465    -0.032581      92.86
 H      -2.492560    -3.821914     0.360716      24.53
 O      -4.105364    -2.618773     1.007848     329.23
 H      -3.379676    -2.234607     1.404573      32.05
 C      -4.427813    -4.616999    -0.402520      96.53
 O      -4.233703    -5.045807    -1.648101     302.03
 H      -5.004546    -5.492010    -1.972890      31.16
 H      -5.470777    -4.281371    -0.291805      26.02
 H      -4.370358    -5.652120     0.336823      23.36
55
name = lig-etoh-frame_178
 C       3.224728     1.361689    -2.005427      88.36
 H       2.852626     2.124112    -2.669704      26.72
 C       4.036265     0.821315     0.152491      56.16
 H       3.902735     1.199073     1.197502      22.75
 C       4.811957    -0.272483    -0.328584      19.81
 O       5.819546    -1.043523     0.291637     171.77
 C       5.591326    -1.011976     1.893910      91.57
 H       4.634101    -0.877848     2.262062      27.94
 H       6.298461    -0.144634     2.186981      26.01
 H       5.985421    -2.089095     2.295955      25.69
 C       4.621363    -0.553448    -1.778315      22.27
 O       5.231257    -1.628563    -2.508571     218.06
 H       5.398121    -2.190819    -1.750382      26.46
 C       3.926149     0.300992    -2.565831      57.71
 H       3.802593    -0.088571    -3.559907      23.34
 C       3.254559     1.628520    -0.673353      40.44
 C       2.364962     2.845895    -0.050119     113.91
 H       2.837311     3.660837    -0.510660      23.71
 O       2.646922     2.818260     1.416679     337.56
 H       3.178094     3.559409     1.618123      29.22
 C       0.892208     2.955228    -0.448325      84.16
 H       0.689379     2.955682    -1.589857      22.25
 C       0.379285     4.446142    -0.028486      81.85
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 O       1.187629     5.626003    -0.502093     226.43
 H       1.338228     5.488994    -1.397622      32.19
 H       0.423057     4.552343     1.181418      23.28
 H      -0.717903     4.328891    -0.307876      23.85
 C      -0.831388    -1.360735    -0.851907      42.28
 H      -0.339172    -2.112836    -1.297390      26.20
 C      -2.954196     0.001762    -0.474399      29.99
 H      -4.062452     0.242927    -0.464609      24.59
 C      -2.222815     1.194806     0.131632     -10.18
 O      -2.841159     2.508544     0.087312     187.42
 C      -4.079189     2.619236     0.695654     121.49
 H      -4.918279     2.338553    -0.068938      24.97
 H      -4.236362     1.965164     1.624918      25.70
 H      -3.914758     3.587627     1.217366      25.15
 C      -0.837875     1.111672    -0.186001      -8.64
 O      -0.027008     2.201024     0.402999     135.91
 C      -0.173092    -0.257167    -0.365675      28.97
 H       0.959294    -0.376146    -0.572158      24.19
 C      -2.310997    -1.239939    -0.776130      29.07
 C      -3.089070    -2.280557    -1.210729      97.40
 H      -3.998693    -2.064215    -1.579647      26.99
 O      -2.290609    -3.216025    -2.169698     211.40
 H      -2.793840    -3.937600    -2.055881      27.25
 C      -3.520832    -3.351470    -0.042624      85.42
 H      -2.552945    -3.729965     0.266704      25.52
 O      -4.125424    -2.621361     1.010574     289.73
 H      -3.256274    -2.456943     1.695997      23.40
 C      -4.475688    -4.626707    -0.380235      99.86
 O      -4.169043    -5.073251    -1.637026     326.16
 H      -4.778045    -5.576745    -2.174994      31.98
 H      -5.573969    -4.317572    -0.255054      26.22
 H      -4.210891    -5.390429     0.381628      26.28
55
name = lig-etoh-frame_179
 C       3.170059     1.332598    -2.045668      71.61
 H       2.717351     2.107335    -2.669664      24.93
 C       3.977381     0.834063     0.240479      70.03
 H       4.247153     1.228440     1.234761      23.93
 C       4.786747    -0.319271    -0.411745      25.11
 O       5.746165    -1.027816     0.281481     160.69
 C       5.653355    -1.081581     1.899751      93.03
 H       4.556249    -0.616682     2.055108      23.98
 H       6.389745    -0.348198     2.044154      27.47
 H       5.998630    -1.990288     2.233050      28.02
 C       4.719044    -0.531064    -1.764156      31.67
 O       5.200438    -1.619437    -2.490714     182.41
 H       5.314629    -2.317633    -1.638220      21.57
 C       3.946563     0.285605    -2.543128      42.22
 H       4.000826     0.159907    -3.675791      21.94
 C       3.251086     1.628390    -0.627815      33.96
 C       2.468059     2.882276    -0.012190     119.92
 H       2.932198     3.727060    -0.779564      21.55
 O       2.661612     2.860786     1.377091     314.89
 H       3.442243     3.537257     1.635056      24.03
 C       0.874768     2.987753    -0.509893      77.76
 H       0.776077     2.935603    -1.572975      22.32
 C       0.447390     4.486175    -0.063741     106.25
 O       1.135286     5.595393    -0.436047     229.43
 H       1.336778     5.415668    -1.489006      26.49
 H       0.586121     4.310072     0.922247      26.07
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 H      -0.615055     4.539378    -0.451887      23.88
 C      -0.892483    -1.396449    -0.819913      50.93
 H      -0.316692    -2.254729    -1.326324      23.26
 C      -2.957621    -0.017952    -0.537734      16.23
 H      -3.992891     0.197848    -0.658419      23.92
 C      -2.243017     1.217796     0.095473     -32.11
 O      -2.796294     2.486720     0.030707     148.33
 C      -4.142103     2.633171     0.801701     110.91
 H      -5.040835     2.654870     0.146320      26.71
 H      -4.370873     2.025095     1.659420      27.09
 H      -4.375797     3.605862     1.358257      26.40
 C      -0.746960     1.171291    -0.216037     -18.64
 O      -0.013368     2.212447     0.358943     159.22
 C      -0.196079    -0.182213    -0.357704      21.27
 H       0.928026     0.140858    -0.453773      22.55
 C      -2.250567    -1.232772    -0.734697      30.95
 C      -3.111288    -2.358863    -1.209031      73.96
 H      -4.030039    -1.772605    -1.854968      23.09
 O      -2.293223    -3.182574    -2.159147     158.97
 H      -2.973593    -4.090186    -2.091541      16.91
 C      -3.584157    -3.337781    -0.055065      92.17
 H      -2.578600    -3.770071     0.213813      23.27
 O      -4.124520    -2.623245     1.045029     307.21
 H      -3.584474    -2.549783     1.855662      28.57
 C      -4.539258    -4.580865    -0.315966      78.42
 O      -4.079301    -5.113492    -1.678656     278.78
 H      -4.713242    -5.677962    -2.322092      28.35
 H      -5.560571    -4.347298    -0.215265      27.54
 H      -4.031780    -5.196492     0.627903      24.09
55
name = lig-etoh-frame_180
 C       3.132608     1.328175    -2.052217      38.86
 H       2.509635     1.943442    -2.721661      22.20
 C       3.980952     0.791089     0.282199      61.34
 H       4.562936     1.097365     1.225950      23.23
 C       4.741550    -0.296964    -0.411807      21.82
 O       5.673179    -1.044343     0.309054     177.19
 C       5.689881    -1.088920     1.815175     109.26
 H       4.769063    -0.705397     2.072350      26.61
 H       6.533169    -0.388341     2.188797      26.71
 H       5.918259    -2.191081     2.208565      25.92
 C       4.796800    -0.530531    -1.777840      34.18
 O       5.187860    -1.636477    -2.427637     241.60
 H       5.400795    -2.438263    -2.011124      26.29
 C       3.930415     0.323353    -2.580683      49.15
 H       4.135348     0.344840    -3.616999      27.06
 C       3.201499     1.638286    -0.587347      21.86
 C       2.570313     2.880085    -0.080087     133.93
 H       2.964395     3.764493    -0.460644      25.75
 O       2.680585     2.939793     1.346903     328.51
 H       3.523806     3.427397     1.484291      27.33
 C       0.910010     3.066005    -0.516071      65.30
 H       0.832266     2.682478    -1.596208      22.16
 C       0.464174     4.452655    -0.097967      99.31
 O       1.127074     5.581569    -0.416809     263.63
 H       1.201310     5.672479    -1.394131      29.23
 H       0.544574     4.252305     1.111383      22.82
 H      -0.576993     4.732178    -0.349672      23.11
 C      -0.889969    -1.335820    -0.753981      52.15
 H      -0.506961    -2.376884    -1.010461      24.91
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 C      -2.905625     0.047289    -0.520565      46.25
 H      -4.038143    -0.100729    -0.894558      25.36
 C      -2.227348     1.181658    -0.067837      -1.25
 O      -2.793909     2.471181     0.019392     108.52
 C      -4.219455     2.677774     0.912167      80.42
 H      -5.069721     2.742798     0.169370      25.47
 H      -4.291424     1.738789     1.586183      24.84
 H      -4.369634     3.694953     1.267614      25.68
 C      -0.738772     1.165758    -0.158734       3.07
 O       0.010369     2.220250     0.289164     174.43
 C      -0.187550    -0.060609    -0.394063      51.10
 H       0.884686     0.114468    -0.347089      23.70
 C      -2.248943    -1.220340    -0.715921       8.11
 C      -3.173746    -2.446915    -1.265783      97.52
 H      -3.802463    -1.921451    -1.821018      27.16
 O      -2.338747    -3.168588    -2.131225     263.41
 H      -2.712008    -3.982228    -2.434461      24.29
 C      -3.612796    -3.316263    -0.063979     105.67
 H      -2.693324    -3.838016     0.188531      23.32
 O      -4.158592    -2.622757     1.086749     305.83
 H      -3.585241    -2.566425     1.850346      29.20
 C      -4.531168    -4.529137    -0.260017      81.16
 O      -3.997450    -5.155238    -1.706732     290.89
 H      -4.706071    -5.594678    -2.158524      32.58
 H      -5.708652    -4.386603    -0.253252      25.90
 H      -4.287429    -5.196822     0.514084      28.02
55
name = lig-etoh-frame_181
 C       3.104308     1.335178    -2.001028      38.90
 H       2.390058     1.770678    -2.695450      22.73
 C       4.031934     0.740524     0.249102      67.95
 H       4.446479     1.017209     1.158950      25.23
 C       4.704583    -0.245945    -0.342442      23.34
 O       5.617431    -1.089643     0.353679     221.60
 C       5.750221    -1.090804     1.706928     137.68
 H       4.743505    -0.807144     2.353972      25.32
 H       6.485098    -0.564507     2.295600      28.72
 H       5.689273    -2.139422     1.994321      27.73
 C       4.785934    -0.506471    -1.801434      14.78
 O       5.202189    -1.671106    -2.400176     199.49
 H       5.536400    -2.558241    -2.077783      23.11
 C       3.938718     0.372992    -2.613342      54.06
 H       4.125447     0.353308    -3.737838      25.96
 C       3.163922     1.608530    -0.583449      41.47
 C       2.599550     2.879262    -0.153562     114.58
 H       3.138043     3.952817    -0.307973      20.98
 O       2.699564     3.021878     1.325742     296.05
 H       3.536804     3.487856     1.434937      27.96
 C       0.987273     3.101575    -0.531822      69.89
 H       0.869588     2.652532    -1.503989      24.26
 C       0.416781     4.385384    -0.065882     108.54
 O       1.175012     5.613626    -0.420966     247.64
 H       1.031272     5.860605    -1.357774      29.51
 H       0.413247     4.461557     0.946683      27.17
 H      -0.713807     4.571292    -0.173182      24.56
 C      -0.856715    -1.221805    -0.655153      27.66
 H      -0.484180    -2.249162    -0.683501      22.88
 C      -2.886691     0.061657    -0.508270      59.09
 H      -3.838499    -0.015915    -0.795678      23.90
 C      -2.200966     1.193872    -0.263711      22.14
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 O      -2.831434     2.468206     0.040966     108.75
 C      -4.277432     2.690638     0.971765      76.03
 H      -4.986159     2.538526     0.094502      24.04
 H      -4.196849     1.778177     1.469212      26.17
 H      -3.923933     3.715211     1.384878      24.07
 C      -0.800248     1.147074    -0.077115      20.23
 O       0.039466     2.238409     0.235489     166.63
 C      -0.141566     0.000032    -0.459944      31.06
 H       1.013688    -0.308085    -0.256274      21.82
 C      -2.299435    -1.218122    -0.725986       3.65
 C      -3.194638    -2.486374    -1.281308      71.87
 H      -4.176858    -1.990034    -1.943968      22.01
 O      -2.351101    -3.162941    -2.127418     256.50
 H      -2.670142    -3.955464    -2.610616      23.32
 C      -3.633111    -3.314973    -0.049083     102.36
 H      -2.671103    -3.819010     0.243973      23.07
 O      -4.214535    -2.619406     1.120970     266.09
 H      -3.260728    -2.488884     1.706220      22.42
 C      -4.525661    -4.490785    -0.281476      91.44
 O      -3.937304    -5.182886    -1.687471     285.42
 H      -4.792140    -5.524433    -1.997659      31.67
 H      -5.536062    -4.319257    -0.445056      26.76
 H      -4.570595    -5.502603     0.459871      24.23
55
name = lig-etoh-frame_182
 C       3.091508     1.324010    -1.945026      66.46
 H       2.329567     1.807274    -2.581049      23.91
 C       4.043592     0.777149     0.190154      60.75
 H       4.085477     1.069903     1.346085      21.87
 C       4.738646    -0.270365    -0.334185      30.20
 O       5.566068    -1.131226     0.353506     246.30
 C       5.730568    -1.112143     1.698144     133.95
 H       4.950136    -0.848795     2.314432      28.15
 H       6.648205    -0.624713     2.167213      27.56
 H       5.766533    -2.264301     1.882807      26.39
 C       4.704487    -0.477627    -1.794782      11.52
 O       5.225058    -1.698110    -2.409851     147.43
 H       5.657319    -2.442164    -1.725120      21.78
 C       3.987330     0.401094    -2.631743      52.28
 H       3.902676     0.254447    -3.693235      22.48
 C       3.164244     1.540814    -0.613585      54.11
 C       2.575413     2.949285    -0.159350     102.68
 H       3.129173     3.684118    -0.664142      24.51
 O       2.708661     3.086032     1.309503     294.95
 H       3.543365     3.744605     1.486455      24.12
 C       1.075186     3.073252    -0.545496      68.68
 H       0.903638     2.942932    -1.665994      23.45
 C       0.351053     4.397279    -0.039313      85.51
 O       1.225412     5.635960    -0.433238     170.68
 H       0.785992     5.906526    -1.391558      25.72
 H       0.464669     4.508281     1.149630      23.56
 H      -0.704374     4.266676    -0.311732      24.50
 C      -0.876877    -1.127399    -0.564721      33.78
 H      -0.157237    -2.072221    -0.402925      21.58
 C      -2.900758     0.000579    -0.530003      21.92
 H      -4.116079     0.332425    -0.619155      19.77
 C      -2.194304     1.304722    -0.390422       8.40
 O      -2.873895     2.466227     0.060542     135.92
 C      -4.246929     2.672102     0.953754      87.54
 H      -5.013705     2.605279     0.234507      24.94
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 H      -4.245636     1.813755     1.745347      25.22
 H      -3.794012     3.447330     1.491373      25.45
 C      -0.797379     1.169583    -0.041955      -2.19
 O       0.053230     2.249403     0.228462     140.04
 C      -0.062377    -0.047079    -0.498125      34.54
 H       0.877471    -0.285894    -0.280751      25.08
 C      -2.333877    -1.211940    -0.758842      39.39
 C      -3.247616    -2.439097    -1.277353      84.24
 H      -4.151122    -2.258022    -1.673115      27.53
 O      -2.317092    -3.161740    -2.151927     197.37
 H      -2.953207    -3.975896    -2.548922      20.12
 C      -3.633026    -3.349820     0.002026      91.77
 H      -2.647094    -3.683044     0.346731      25.91
 O      -4.223183    -2.616054     1.151884     307.94
 H      -3.462655    -2.239950     1.489205      30.77
 C      -4.514877    -4.540313    -0.362630      92.51
 O      -3.910527    -5.196545    -1.628959     286.13
 H      -4.854835    -5.510889    -2.005574      28.72
 H      -5.551406    -4.044442    -0.756373      24.80
 H      -4.582783    -5.262151     0.301070      28.08
55
name = lig-etoh-frame_183
 C       3.098032     1.284753    -1.973848      66.46
 H       2.402063     1.946935    -2.473465      23.50
 C       4.030445     0.857591     0.193592      60.95
 H       3.772514     1.009549     1.173309      24.60
 C       4.791669    -0.308930    -0.387005      20.93
 O       5.519821    -1.176157     0.298564     214.14
 C       5.724067    -1.191331     1.770015     110.19
 H       4.796162    -0.687618     2.325944      24.30
 H       6.667015    -0.652247     1.827575      27.19
 H       6.056680    -2.238219     1.965865      26.40
 C       4.634182    -0.504737    -1.783369      15.70
 O       5.250141    -1.695570    -2.395738     224.59
 H       5.559835    -1.992951    -1.605028      27.37
 C       4.003131     0.422078    -2.613269      53.04
 H       3.725073     0.114747    -3.648797      22.44
 C       3.166675     1.521254    -0.613114      37.92
 C       2.532220     2.967623    -0.128631      99.50
 H       3.086636     3.530080    -1.044175      22.00
 O       2.727088     3.162091     1.284246     327.15
 H       3.318280     3.884069     1.421456      28.07
 C       1.108958     3.065675    -0.551645      70.23
 H       0.981722     3.278795    -1.620651      23.03
 C       0.359451     4.447797     0.010881      94.27
 O       1.220652     5.630105    -0.466962     208.14
 H       0.862906     5.864034    -1.284270      31.47
 H       0.427133     4.347301     1.032020      26.27
 H      -0.610538     4.244395    -0.545665      24.00
 C      -0.903615    -1.149953    -0.500954      40.27
 H      -0.289481    -1.942501    -0.410514      23.31
 C      -2.986463     0.043483    -0.574298      15.99
 H      -3.932130     0.275210    -0.436258      21.78
 C      -2.209148     1.379277    -0.420676      -6.31
 O      -2.920844     2.473850     0.069221     184.40
 C      -4.126500     2.570094     0.930321     106.01
 H      -5.199070     2.922302     0.448252      24.55
 H      -4.431511     1.958652     1.774387      26.37
 H      -3.937354     3.555300     1.556100      25.41
 C      -0.712101     1.212363    -0.107451     -10.81
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 O       0.063340     2.252007     0.255010     118.71
 C      -0.066405    -0.049249    -0.479977      21.31
 H       1.167669    -0.060512    -0.250495      20.77
 C      -2.362122    -1.207788    -0.802018      34.16
 C      -3.224177    -2.393672    -1.202210      60.04
 H      -4.369980    -2.171337    -1.693712      23.32
 O      -2.312773    -3.169357    -2.189648     216.71
 H      -2.905209    -3.837959    -2.276902      27.32
 C      -3.593395    -3.383955     0.067325      83.84
 H      -2.615517    -3.710299     0.454899      25.70
 O      -4.236880    -2.624211     1.149721     270.52
 H      -3.541177    -1.897305     1.555057      25.08
 C      -4.512733    -4.543854    -0.517158      99.53
 O      -3.926639    -5.208973    -1.559346     335.00
 H      -4.562061    -5.553635    -2.167297      31.86
 H      -5.347103    -4.017762    -0.803312      28.19
 H      -4.689524    -5.255652     0.548849      24.58
55
name = lig-etoh-frame_184
 C       3.105002     1.278185    -2.031044      66.39
 H       2.537439     2.015088    -2.623073      24.22
 C       4.046943     0.858013     0.196888      53.91
 H       3.766760     0.937952     1.340373      22.43
 C       4.775207    -0.256830    -0.426706      19.00
 O       5.493320    -1.264668     0.253626     196.78
 C       5.722150    -1.254116     1.813233     112.72
 H       4.888012    -0.755593     2.279833      26.45
 H       6.505957    -0.495977     1.819466      27.36
 H       6.052050    -2.226581     2.169695      27.33
 C       4.613452    -0.572159    -1.799979      15.92
 O       5.254607    -1.638228    -2.362181     184.55
 H       5.704157    -1.990419    -1.443844      19.61
 C       3.957393     0.411044    -2.602179      61.71
 H       3.764040     0.038646    -3.618670      23.10
 C       3.148382     1.571889    -0.608385      41.03
 C       2.513281     2.909164    -0.140547     113.58
 H       2.976294     3.616170    -0.774378      24.36
 O       2.728719     3.235555     1.241659     302.84
 H       3.324591     4.087235     1.324152      25.40
 C       1.066131     3.136334    -0.509515      75.19
 H       0.972855     3.167945    -1.614573      23.37
 C       0.447262     4.481388    -0.008004     102.02
 O       1.185315     5.599778    -0.476026     227.70
 H       0.949980     5.836714    -1.446549      27.51
 H       0.288012     4.353047     1.165798      23.89
 H      -0.542773     4.601258    -0.392986      25.24
 C      -0.947899    -1.215535    -0.487419      15.97
 H      -0.505332    -2.392499    -0.565723      18.55
 C      -3.001226     0.166856    -0.624418      24.64
 H      -4.254184     0.089590    -0.393082      21.16
 C      -2.220502     1.346086    -0.375768      -8.93
 O      -2.965878     2.497193     0.071664     218.17
 C      -4.035459     2.538771     0.933188     136.29
 H      -4.899362     2.907922     0.500941      27.86
 H      -4.377854     1.704619     1.624159      26.88
 H      -3.991324     3.475083     1.418647      27.58
 C      -0.658712     1.253994    -0.256180      -6.74
 O       0.090024     2.261186     0.288644     152.01
 C      -0.089528     0.004340    -0.402270      46.55
 H       0.886784     0.041519    -0.351951      25.23
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 C      -2.373402    -1.146917    -0.816846      10.88
 C      -3.182495    -2.377872    -1.114949      85.52
 H      -3.972788    -1.980977    -1.585998      27.16
 O      -2.336032    -3.144451    -2.204165     151.04
 H      -2.825208    -4.136965    -2.176745      19.45
 C      -3.517326    -3.386162     0.107098      93.71
 H      -2.610894    -3.913473     0.509040      25.08
 O      -4.256112    -2.640055     1.128072     294.78
 H      -3.650701    -1.899520     1.542707      26.88
 C      -4.517577    -4.517780    -0.542947     105.58
 O      -3.918547    -5.246339    -1.526896     331.70
 H      -4.376853    -5.584075    -2.308229      30.73
 H      -5.540840    -3.978234    -0.869617      25.57
 H      -4.843513    -5.046632     0.211728      29.21
55
name = lig-etoh-frame_185
 C       3.091613     1.353464    -2.043206      61.42
 H       2.657152     1.951960    -2.848934      24.67
 C       4.045710     0.810870     0.210629      64.29
 H       4.157285     0.874445     1.263173      23.78
 C       4.726978    -0.195004    -0.419770      16.34
 O       5.472481    -1.371733     0.241619     164.22
 C       5.728798    -1.264689     1.777686     109.58
 H       4.767021    -0.958521     2.354392      25.41
 H       6.395439    -0.401775     2.085049      26.89
 H       5.933276    -2.291039     2.337323      25.63
 C       4.608258    -0.584978    -1.813450      24.94
 O       5.269485    -1.581588    -2.298290     203.62
 H       5.831315    -2.239223    -1.780524      22.83
 C       3.902055     0.311397    -2.620945      54.95
 H       3.906523     0.130666    -3.701341      21.79
 C       3.139803     1.633906    -0.632468      47.48
 C       2.498133     2.856216    -0.151940     119.65
 H       3.035479     3.877304    -0.577200      18.79
 O       2.715365     3.300098     1.207592     282.49
 H       3.445240     4.017760     1.182255      25.03
 C       0.969185     3.214200    -0.456517      76.88
 H       0.821989     2.808998    -1.501913      21.88
 C       0.521221     4.506148    -0.024923     113.74
 O       1.164231     5.597254    -0.479716     248.00
 H       1.102155     5.612447    -1.548575      26.17
 H       0.380802     4.628698     1.031435      24.73
 H      -0.599100     4.795406    -0.224353      22.18
 C      -0.989609    -1.288792    -0.526862      44.18
 H      -0.779299    -2.231810    -0.669536      23.64
 C      -3.018564     0.260221    -0.665730      70.98
 H      -3.998209     0.094267    -0.603956      26.93
 C      -2.236572     1.296755    -0.286065     -23.02
 O      -2.939799     2.515740     0.036621     186.37
 C      -4.005055     2.528232     0.972176      91.16
 H      -4.926924     2.631048     0.132469      22.53
 H      -4.035497     1.467061     1.342086      25.54
 H      -3.738672     3.418330     1.700210      23.49
 C      -0.701374     1.302792    -0.404879      -5.59
 O       0.123440     2.274629     0.309324     158.69
 C      -0.185706    -0.004437    -0.326529      10.05
 H       1.054400    -0.080206    -0.356222      21.05
 C      -2.328569    -1.040070    -0.777690       4.37
 C      -3.074339    -2.393481    -1.037333      73.87
 H      -4.055619    -1.862212    -1.596768      21.52
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 O      -2.397265    -3.124044    -2.191680     209.96
 H      -2.444849    -4.111703    -2.090913      21.63
 C      -3.466212    -3.375818     0.099634     100.50
 H      -2.667311    -3.998044     0.499095      24.39
 O      -4.276961    -2.668695     1.093662     335.75
 H      -3.634562    -2.146747     1.506741      31.84
 C      -4.573895    -4.404807    -0.524067      78.76
 O      -3.865428    -5.312825    -1.529303     277.89
 H      -4.476620    -5.469059    -2.401510      28.14
 H      -5.416525    -3.967238    -0.976920      26.03
 H      -5.082108    -5.258356     0.307048      23.56
55
name = lig-etoh-frame_186
 C       3.112739     1.412140    -2.052434      52.25
 H       2.618807     1.990591    -2.832931      20.45
 C       4.011751     0.787748     0.199507      62.59
 H       4.422825     0.990364     1.248384      22.66
 C       4.704435    -0.233554    -0.401359       6.94
 O       5.450113    -1.445598     0.273746     158.49
 C       5.686956    -1.250339     1.738760     127.49
 H       4.671890    -1.260372     2.201541      26.36
 H       6.369772    -0.536188     2.181783      28.20
 H       5.981192    -2.188439     2.093306      29.07
 C       4.598593    -0.526329    -1.764375      24.91
 O       5.313745    -1.577242    -2.290745     224.06
 H       5.738066    -2.282364    -1.902628      25.57
 C       3.821874     0.209783    -2.645182      56.05
 H       4.024350     0.276198    -3.748639      28.43
 C       3.164209     1.660749    -0.670933      31.72
 C       2.478199     2.938330    -0.160710     120.88
 H       2.942644     3.690149    -0.742645      25.54
 O       2.694756     3.333471     1.202281     330.40
 H       3.548343     3.807515     1.217725      27.64
 C       0.893629     3.169504    -0.435136      83.60
 H       0.650418     2.851956    -1.433901      23.03
 C       0.480754     4.575649    -0.014130     105.94
 O       1.198628     5.642493    -0.531709     296.49
 H       1.225683     5.492956    -1.429486      33.12
 H       0.720784     4.719153     1.137899      23.51
 H      -0.577128     4.542172    -0.217438      25.27
 C      -1.008771    -1.224509    -0.574878      43.78
 H      -0.589857    -2.394832    -0.719251      20.34
 C      -2.979363     0.247259    -0.709768      47.95
 H      -4.217684     0.314715    -0.800584      23.02
 C      -2.230570     1.346153    -0.198190     -21.10
 O      -2.840579     2.537343    -0.023836     190.47
 C      -4.002664     2.499133     0.969436     111.87
 H      -4.839066     2.476308     0.441321      27.98
 H      -3.871205     1.490979     1.329476      27.81
 H      -3.783783     3.034313     1.850712      26.71
 C      -0.788674     1.326115    -0.466017     -12.15
 O       0.126287     2.268971     0.324471     165.50
 C      -0.246468    -0.083597    -0.297600       6.74
 H       0.767136    -0.211237    -0.197865      22.71
 C      -2.301632    -0.972585    -0.717951      25.09
 C      -3.011158    -2.372271    -1.035046      93.72
 H      -3.980596    -2.211344    -1.311216      25.30
 O      -2.445622    -3.085555    -2.160380     259.56
 H      -2.337094    -4.006817    -1.910663      22.96
 C      -3.494423    -3.383746     0.059599      96.68
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 H      -2.654791    -3.986274     0.526598      23.56
 O      -4.283091    -2.701909     1.050606     296.38
 H      -3.480321    -2.326564     1.764974      22.15
 C      -4.606486    -4.357339    -0.488431      83.23
 O      -3.829072    -5.371652    -1.541632     320.14
 H      -4.464218    -5.235583    -2.203014      31.53
 H      -5.362261    -3.732412    -1.141530      25.75
 H      -4.960064    -4.956799     0.177118      27.77
55
name = lig-etoh-frame_187
 C       3.168275     1.396000    -2.087094      45.42
 H       2.505264     2.121406    -2.611145      19.13
 C       3.973583     0.800670     0.186112      52.49
 H       4.320207     1.273175     1.133842      22.30
 C       4.700271    -0.356824    -0.356442       9.71
 O       5.422451    -1.451471     0.314761     202.88
 C       5.599023    -1.277258     1.692980     112.21
 H       4.590841    -1.275919     2.131090      25.35
 H       6.343143    -0.478134     2.055019      25.72
 H       6.269386    -2.299522     1.788025      24.38
 C       4.608730    -0.511610    -1.730340       8.19
 O       5.357067    -1.566707    -2.336435     167.70
 H       5.567928    -2.351035    -1.614492      21.42
 C       3.725777     0.202701    -2.645157      57.60
 H       4.000367     0.191203    -3.676920      27.25
 C       3.203770     1.668705    -0.681181      16.39
 C       2.439152     3.042566    -0.183605      83.57
 H       2.903955     3.753583    -1.093579      20.94
 O       2.667778     3.341216     1.205302     307.22
 H       3.666395     3.661559     1.385689      25.28
 C       0.872632     3.090886    -0.433621      76.99
 H       0.618674     3.173733    -1.566645      20.20
 C       0.415690     4.631620     0.054113      92.71
 O       1.246524     5.698255    -0.603316     193.22
 H       1.325312     5.547185    -1.682247      25.35
 H       0.872164     4.572266     1.039201      23.73
 H      -0.688762     4.504783    -0.166076      23.57
 C      -0.945408    -1.164942    -0.612901      64.51
 H      -0.445652    -2.025285    -0.596770      24.47
 C      -2.970272     0.213942    -0.717056      42.01
 H      -3.934975     0.540746    -1.006825      25.33
 C      -2.191483     1.417015    -0.189298      -3.89
 O      -2.755467     2.601322    -0.058736     180.89
 C      -3.941192     2.409555     0.958685      81.21
 H      -5.161070     2.601661     0.665152      23.16
 H      -3.897040     1.374134     1.459163      25.36
 H      -3.906844     3.038549     1.943939      24.50
 C      -0.841080     1.283122    -0.396605      13.06
 O       0.079933     2.224885     0.340385     171.57
 C      -0.294866    -0.106544    -0.311204      22.72
 H       0.846066    -0.238288     0.018014      20.82
 C      -2.383908    -1.013922    -0.694960      26.57
 C      -3.011711    -2.337976    -1.045656      77.97
 H      -4.193904    -2.173134    -1.301374      21.75
 O      -2.469595    -3.034785    -2.135520     213.22
 H      -2.323680    -4.028062    -1.686821      17.86
 C      -3.529655    -3.413306     0.036500     108.98
 H      -2.721726    -3.942099     0.501119      24.26
 O      -4.248010    -2.711530     1.045929     321.49
 H      -3.735494    -2.574259     1.795306      29.90
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 C      -4.556675    -4.314007    -0.539565      66.95
 O      -3.828101    -5.395909    -1.525171     293.90
 H      -4.419646    -5.151122    -2.302983      28.92
 H      -5.234703    -3.668395    -1.104423      26.20
 H      -5.086803    -4.911661     0.453409      23.98
55
name = lig-etoh-frame_188
 C       3.189462     1.373861    -2.099315      48.20
 H       2.539464     2.094264    -2.556087      20.51
 C       3.959438     0.824588     0.166343      51.12
 H       4.054581     1.341294     1.132783      21.54
 C       4.666167    -0.458012    -0.296387      20.08
 O       5.376599    -1.403248     0.309386     239.87
 C       5.561108    -1.357820     1.667668     131.82
 H       4.609552    -1.270638     2.331479      25.70
 H       6.052889    -0.399084     1.809899      27.51
 H       6.190567    -2.112676     1.855837      29.72
 C       4.617044    -0.557819    -1.758176       2.78
 O       5.392898    -1.555807    -2.369792     206.49
 H       5.320937    -2.145646    -1.587525      23.53
 C       3.683207     0.238470    -2.600670      57.35
 H       3.800876    -0.064391    -3.697483      25.31
 C       3.242946     1.672056    -0.679300      27.44
 C       2.426254     3.097476    -0.248585      91.94
 H       2.720014     3.881190    -0.919745      22.69
 O       2.645207     3.336565     1.198307     335.40
 H       3.512794     3.686702     1.368769      28.86
 C       0.871055     3.090171    -0.453185      73.33
 H       0.698959     3.225263    -1.487232      21.23
 C       0.402899     4.637759     0.081984      80.28
 O       1.272442     5.720052    -0.683227     189.86
 H       1.137983     5.693003    -1.666213      27.94
 H       0.697142     4.627358     1.148829      24.54
 H      -0.707459     4.864348     0.038349      24.40
 C      -0.957473    -1.149082    -0.643222      25.48
 H      -0.300178    -2.149380    -0.496361      22.99
 C      -2.937079     0.243341    -0.682285      37.46
 H      -3.978054     0.527619    -1.157674      25.47
 C      -2.153579     1.412134    -0.277576       2.00
 O      -2.740295     2.697184    -0.043587     181.50
 C      -3.915071     2.327839     0.988735     105.12
 H      -4.803495     2.647500     0.663770      27.97
 H      -3.910747     1.341760     1.318651      29.05
 H      -3.749337     3.140377     1.669644      26.52
 C      -0.807982     1.213580    -0.220138      31.66
 O       0.011434     2.159908     0.340636     184.38
 C      -0.237341     0.003167    -0.325280      40.69
 H       0.765379    -0.073212     0.142930      21.31
 C      -2.444662    -1.119308    -0.708546       9.73
 C      -3.157260    -2.307527    -1.053342      88.78
 H      -4.002566    -1.823109    -1.457734      22.73
 O      -2.459039    -3.009165    -2.113338     242.16
 H      -2.369230    -3.885917    -1.857995      22.73
 C      -3.517960    -3.405989     0.042572     105.77
 H      -2.653095    -4.024828     0.457237      21.96
 O      -4.237827    -2.713374     1.050228     309.43
 H      -3.685546    -2.659391     1.915999      24.55
 C      -4.489768    -4.355341    -0.591724      98.34
 O      -3.877100    -5.374706    -1.488215     324.72
 H      -4.160729    -5.264897    -2.503165      28.85
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 H      -5.284616    -3.742279    -1.135860      26.51
 H      -5.054084    -4.689761     0.176070      28.23
55
name = lig-etoh-frame_189
 C       3.153159     1.405213    -2.055828      26.83
 H       2.594452     2.002016    -2.829414      20.43
 C       3.976093     0.823947     0.167524      69.16
 H       3.805021     1.058394     1.297355      20.99
 C       4.557024    -0.436619    -0.320373      20.95
 O       5.326620    -1.383879     0.274192     217.01
 C       5.525305    -1.380907     1.695285     118.92
 H       4.692753    -1.456057     2.366788      27.39
 H       5.874331    -0.304934     1.824708      26.03
 H       6.270548    -2.221840     2.189383      25.46
 C       4.591928    -0.594523    -1.786470      13.38
 O       5.401488    -1.533434    -2.383377     227.57
 H       5.433939    -2.300582    -1.786720      24.11
 C       3.738326     0.207775    -2.569902      55.17
 H       3.430096    -0.182025    -3.531011      25.32
 C       3.261501     1.701213    -0.713748      43.41
 C       2.426501     3.065233    -0.264187      99.47
 H       2.754392     4.153830    -0.793567      19.35
 O       2.607453     3.317860     1.170548     276.94
 H       3.466202     3.907465     1.252306      25.50
 C       0.847937     3.159097    -0.442218      42.88
 H       0.620791     2.950257    -1.572892      20.85
 C       0.432324     4.638336     0.073454      91.74
 O       1.266384     5.709283    -0.716855     154.84
 H       0.857948     5.680694    -1.683073      25.25
 H       0.555860     4.867311     1.198793      24.56
 H      -0.569669     5.077812     0.033493      24.75
 C      -0.996096    -1.167890    -0.638793      36.96
 H      -0.528163    -2.157568    -0.558306      22.07
 C      -2.919058     0.278375    -0.655501      45.60
 H      -3.971891     0.302466    -1.070449      21.01
 C      -2.166117     1.392733    -0.406186     -15.06
 O      -2.755732     2.738731    -0.008598     169.42
 C      -3.849232     2.325876     1.004920      54.34
 H      -4.834097     2.620812     0.285604      21.15
 H      -3.833554     1.181425     1.254200      22.65
 H      -3.472826     3.108717     1.722285      23.47
 C      -0.761838     1.198424    -0.023228      18.20
 O      -0.015539     2.149998     0.349445     181.66
 C      -0.153092     0.039188    -0.345587      35.52
 H       0.879228     0.042527     0.081171      20.46
 C      -2.383135    -1.135559    -0.715319      13.75
 C      -3.320233    -2.307018    -1.071829      67.15
 H      -4.178284    -1.747604    -1.665117      22.03
 O      -2.436678    -2.976690    -2.118554     192.52
 H      -2.440666    -3.988050    -1.987897      20.79
 C      -3.489180    -3.365195     0.036924     107.57
 H      -2.595171    -3.904418     0.306111      25.14
 O      -4.245108    -2.718697     1.079294     296.46
 H      -3.483865    -2.582800     1.860254      22.83
 C      -4.451733    -4.397854    -0.695425      90.34
 O      -3.930713    -5.350931    -1.460309     341.83
 H      -4.028176    -5.269306    -2.358398      33.94
 H      -5.274002    -3.853975    -1.254670      25.60
 H      -5.151366    -4.962367     0.211617      25.87
55
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name = lig-etoh-frame_190
 C       2.611366     1.344386    -2.218244      73.81
 H       2.262306     2.121780    -2.971856      24.62
 C       3.711283     0.704684    -0.158771      57.88
 H       3.515162     0.787447     0.966518      21.68
 C       4.391192    -0.352603    -0.725788       9.38
 O       5.412197    -1.152009    -0.117092     191.20
 C       5.407531    -0.844136     1.282716     114.81
 H       4.384616    -1.150588     1.880499      24.82
 H       5.849696     0.112963     1.496319      26.95
 H       6.064126    -1.757210     1.540819      25.57
 C       4.229884    -0.578350    -2.174239     -11.59
 O       4.642382    -1.828784    -2.944762     131.09
 H       5.344581    -2.440783    -2.451158      21.59
 C       3.414536     0.421552    -2.884769      53.75
 H       3.352337     0.066525    -3.860375      22.84
 C       2.887251     1.659010    -0.874042      25.74
 C       2.417616     2.949104    -0.159176      94.01
 H       2.842455     4.012688    -0.721917      20.71
 O       2.952259     3.006331     1.119057     307.53
 H       3.570139     3.756246     1.306662      27.25
 C       0.834236     3.278431    -0.344496      87.16
 H       0.610061     3.082842    -1.436696      23.08
 C       0.415189     4.690000     0.108542     122.75
 O       0.817538     5.854024    -0.554401     261.51
 H       0.829887     5.714053    -1.564739      28.95
 H       0.684873     4.605775     1.041451      27.92
 H      -0.600848     4.738958     0.293752      27.08
 C      -1.357407    -0.655186    -0.820368      32.97
 H      -0.813289    -1.614179    -1.219857      23.32
 C      -3.144919     0.405028     0.273692      71.52
 H      -4.285704     0.211784     0.373185      19.32
 C      -2.238762     1.431876     0.642829      15.45
 O      -2.720208     2.463399     1.510231     172.25
 C      -4.096495     2.906421     1.162238      93.27
 H      -4.655775     3.495142     2.267819      23.43
 H      -3.951134     3.870366     0.551707      25.20
 H      -4.897147     2.153450     0.937923      24.35
 C      -0.962068     1.550456     0.023099      12.44
 O       0.088670     2.462516     0.636644     138.84
 C      -0.501316     0.412396    -0.538997      36.43
 H       0.634705     0.542261    -1.136734      18.59
 C      -2.782580    -0.666114    -0.515915      18.28
 C      -3.542153    -1.856080    -0.910618      85.09
 H      -4.511032    -1.627708    -1.363534      24.12
 O      -2.908255    -2.645262    -1.984175     290.20
 H      -2.792764    -3.530646    -1.690999      23.59
 C      -3.869095    -3.020123     0.196291      73.00
 H      -2.851884    -3.286274     0.411312      25.15
 O      -4.395716    -2.314895     1.336107     385.12
 H      -3.762985    -2.006362     1.902857      29.97
 C      -4.631194    -4.319997    -0.425602      94.86
 O      -3.921886    -5.030651    -1.403095     335.29
 H      -4.541638    -5.053607    -2.101244      33.17
 H      -5.447345    -3.761650    -0.796037      27.43
 H      -4.955336    -4.954992     0.578743      24.99
55
name = lig-etoh-frame_191
 C       3.122623     1.352048    -2.080498      37.95
 H       2.536320     1.982432    -2.799196      22.76
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 C       3.899794     0.810935     0.182502      66.86
 H       3.793330     0.606413     1.348772      23.40
 C       4.418292    -0.310975    -0.441820      25.43
 O       5.227169    -1.413199     0.265408     137.65
 C       5.439808    -1.336181     1.796131     110.45
 H       4.559538    -1.760464     2.116291      27.45
 H       5.755366    -0.406789     2.378902      25.68
 H       6.390117    -2.108381     1.809507      25.35
 C       4.518818    -0.673901    -1.762044      28.49
 O       5.397823    -1.518516    -2.416293     250.44
 H       5.588426    -2.419957    -2.230693      25.98
 C       3.749660     0.202954    -2.563488      40.55
 H       3.441331    -0.152085    -3.570077      21.64
 C       3.216641     1.839891    -0.705684      47.74
 C       2.425449     2.981414    -0.217554     125.71
 H       2.972017     3.865766    -0.943425      20.15
 O       2.579600     3.272320     1.143091     344.22
 H       3.151779     3.995737     1.278258      29.39
 C       0.782809     3.233227    -0.433694      55.02
 H       0.383182     3.011814    -1.488072      22.10
 C       0.481444     4.716322    -0.043643     112.74
 O       1.203043     5.631974    -0.715072     288.99
 H       0.998444     5.624096    -1.631543      31.15
 H       0.834627     4.724724     1.099176      23.55
 H      -0.563551     4.633713    -0.271883      25.29
 C      -0.902711    -1.193346    -0.552408      34.60
 H      -0.574497    -2.241423    -0.960142      19.25
 C      -2.942821     0.212784    -0.694582      38.99
 H      -4.111776     0.359277    -0.547835      20.28
 C      -2.139967     1.464736    -0.455281     -12.78
 O      -2.736742     2.625139     0.003121     238.69
 C      -3.721061     2.427231     0.964419      83.81
 H      -4.945685     2.523448     0.637529      22.75
 H      -3.611874     1.302949     1.297013      24.37
 H      -3.874976     2.854872     1.989963      24.83
 C      -0.790938     1.177958     0.052351     -31.70
 O       0.085912     2.370826     0.529327     132.66
 C      -0.091246    -0.134798    -0.330609      31.08
 H       0.939070    -0.276271    -0.510419      22.46
 C      -2.382647    -0.959194    -0.755549      25.57
 C      -3.323065    -2.234517    -1.175706      66.07
 H      -4.438460    -2.155241    -1.511003      22.32
 O      -2.433569    -2.945814    -2.166138     238.04
 H      -2.736674    -3.784349    -2.183844      25.27
 C      -3.598689    -3.273304    -0.084559      94.04
 H      -2.595988    -3.557455     0.183229      24.03
 O      -4.212254    -2.772777     1.167855     292.96
 H      -3.531706    -1.987427     1.570925      22.41
 C      -4.583847    -4.385738    -0.649472      73.05
 O      -3.897835    -5.455673    -1.542290     312.16
 H      -4.236386    -5.132532    -2.482399      27.59
 H      -5.397284    -3.813611    -1.278084      25.21
 H      -5.035249    -5.020140     0.272984      25.04
55
name = lig-etoh-frame_192
 C       3.124393     1.336637    -2.083547      50.63
 H       2.452904     1.987440    -2.625010      20.06
 C       3.781569     0.843429     0.160419      46.04
 H       3.844429     0.924027     1.183435      23.23
 C       4.488166    -0.365193    -0.412042      30.42
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 O       5.160857    -1.368871     0.304247     204.84
 C       5.397982    -1.346221     1.778787     117.22
 H       4.486259    -1.905310     2.313973      25.34
 H       5.535706    -0.412304     2.305611      26.70
 H       6.238417    -1.978720     1.728772      28.26
 C       4.476115    -0.695508    -1.794807      30.06
 O       5.397389    -1.506818    -2.458570     228.42
 H       5.361582    -2.444549    -1.994766      25.32
 C       3.687573     0.213389    -2.617154      43.29
 H       3.797792    -0.013937    -3.696574      25.35
 C       3.191910     1.773535    -0.665660      37.63
 C       2.400787     3.009646    -0.238479     124.27
 H       2.831030     3.671919    -0.940907      25.27
 O       2.574977     3.240375     1.170573     321.43
 H       3.295869     3.991789     1.358469      24.53
 C       0.806576     3.191453    -0.438959      82.87
 H       0.453740     3.244943    -1.467338      21.54
 C       0.462084     4.665204    -0.084596     105.99
 O       1.191683     5.639070    -0.726349     257.72
 H       1.283503     5.578124    -1.804148      26.58
 H       0.641403     4.718644     0.916418      26.83
 H      -0.730597     4.674004    -0.026629      24.13
 C      -0.898888    -1.242128    -0.558829      26.75
 H      -0.446364    -2.095780    -0.982839      18.65
 C      -2.994705     0.320265    -0.699749      37.39
 H      -4.001380     0.390395    -0.558458      24.58
 C      -2.078442     1.432038    -0.341650       5.79
 O      -2.706508     2.583346    -0.023954     231.80
 C      -3.754399     2.399982     1.010245      94.79
 H      -4.712442     2.599414     0.669785      26.25
 H      -3.635033     1.411613     1.331396      27.73
 H      -3.616751     3.245889     1.800449      24.76
 C      -0.727206     1.210135    -0.041510     -11.71
 O       0.106997     2.449713     0.635874     127.32
 C      -0.119259    -0.147643    -0.275167      26.02
 H       1.037700    -0.352834    -0.654925      19.74
 C      -2.417815    -0.995795    -0.803666       9.21
 C      -3.231364    -2.187067    -1.222559      91.38
 H      -4.124367    -1.709853    -1.690140      22.48
 O      -2.463443    -2.914994    -2.195561     213.32
 H      -2.863013    -3.936942    -2.253071      16.95
 C      -3.656306    -3.243443    -0.113204      93.65
 H      -2.704561    -3.807321     0.183294      21.73
 O      -4.199683    -2.791558     1.177231     346.47
 H      -3.648792    -2.092693     1.493580      27.43
 C      -4.632131    -4.385097    -0.577567      82.16
 O      -3.882571    -5.481009    -1.627940     288.03
 H      -4.344857    -5.375318    -2.430900      33.02
 H      -5.488750    -3.973236    -1.080837      27.01
 H      -5.122137    -4.746512     0.330915      27.33
55
name = lig-etoh-frame_193
 C       3.090212     1.377682    -2.050122      66.53
 H       2.434564     1.986972    -2.687345      21.10
 C       3.720000     0.800246     0.142794      47.46
 H       3.875159     1.331285     1.209081      20.34
 C       4.533600    -0.405099    -0.368650      11.43
 O       5.096978    -1.312565     0.365811     226.97
 C       5.311244    -1.378488     1.744995     122.13
 H       4.655834    -1.885492     2.377670      27.15
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 H       5.398249    -0.305417     2.096337      24.78
 H       6.336785    -1.980587     1.916195      25.41
 C       4.422782    -0.648639    -1.843676      11.20
 O       5.381405    -1.516737    -2.486666     190.13
 H       5.260300    -2.337919    -1.849297      24.34
 C       3.667455     0.184823    -2.677554      49.89
 H       4.008610     0.247626    -3.751600      26.80
 C       3.125589     1.651367    -0.690137      39.03
 C       2.361926     3.022491    -0.255804     106.76
 H       2.805608     3.976673    -0.939525      20.68
 O       2.589578     3.225834     1.207806     322.91
 H       3.391655     3.796068     1.279758      27.18
 C       0.858232     3.168414    -0.423127      84.91
 H       0.522054     2.960208    -1.486007      19.60
 C       0.392208     4.576742    -0.085592      96.64
 O       1.201820     5.679395    -0.761422     243.10
 H       1.216843     5.385860    -1.699322      30.91
 H       0.616661     4.853774     1.068072      23.28
 H      -0.633083     4.858960    -0.109028      24.61
 C      -0.999440    -1.244841    -0.600581      31.14
 H      -0.269032    -2.177086    -0.944034      17.95
 C      -2.952711     0.390448    -0.687461      21.55
 H      -4.181635     0.535127    -0.763626      22.84
 C      -2.039351     1.346697    -0.203411      -5.39
 O      -2.686048     2.579302    -0.045922     191.10
 C      -3.759150     2.420532     1.072474      74.60
 H      -4.812280     2.638155     0.444798      23.20
 H      -3.737303     1.393095     1.634084      25.15
 H      -3.280021     3.291264     1.525983      22.69
 C      -0.608127     1.249434    -0.120367      -5.27
 O       0.091304     2.461377     0.679266     140.99
 C      -0.121894    -0.102195    -0.239494      30.85
 H       0.867320    -0.163162    -0.357211      22.51
 C      -2.383825    -1.034236    -0.823597      14.00
 C      -3.174825    -2.140346    -1.266817      89.40
 H      -3.895122    -1.462169    -1.876753      19.77
 O      -2.497725    -2.912518    -2.241552     246.25
 H      -2.871536    -3.837154    -2.228200      18.93
 C      -3.681339    -3.250822    -0.111121      87.53
 H      -2.865597    -3.956959     0.037003      20.62
 O      -4.215880    -2.811884     1.147789     304.40
 H      -3.522432    -2.198700     1.611793      22.87
 C      -4.656105    -4.380232    -0.552224      67.73
 O      -3.891411    -5.459450    -1.667982     227.41
 H      -4.602363    -5.585776    -2.447188      30.45
 H      -5.665360    -4.106205    -1.137308      24.24
 H      -5.024410    -4.873847     0.448030      24.96
55
name = lig-etoh-frame_194
 C       3.031457     1.385779    -2.082013      50.14
 H       2.533180     2.045381    -2.803490      20.46
 C       3.751642     0.694383     0.193413      59.53
 H       3.868349     1.280189     1.033873      22.42
 C       4.467924    -0.344827    -0.371587      10.68
 O       5.060909    -1.324418     0.415805     233.91
 C       5.275035    -1.375422     1.742975     128.86
 H       4.458819    -1.950813     2.377799      24.85
 H       5.327448    -0.320645     2.032221      25.22
 H       6.264868    -1.724754     2.069720      27.14
 C       4.413257    -0.592773    -1.867124      13.24
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 O       5.331301    -1.527541    -2.478695     219.57
 H       5.451846    -2.310646    -2.006348      27.01
 C       3.673017     0.217575    -2.708791      57.99
 H       3.921338     0.352221    -3.730288      27.62
 C       2.991646     1.598466    -0.765411      39.84
 C       2.371417     3.025473    -0.255109     118.34
 H       2.748125     3.959677    -0.616620      22.58
 O       2.615923     3.214083     1.223993     326.21
 H       3.471710     3.675593     1.250776      28.51
 C       0.877064     3.160068    -0.394941      70.16
 H       0.619413     2.536045    -1.275777      18.54
 C       0.364517     4.568951    -0.040167      96.15
 O       1.199896     5.693248    -0.779852     186.72
 H       1.021103     5.390281    -1.753953      26.52
 H       0.614238     4.758736     0.938574      25.27
 H      -0.700126     4.850702    -0.487885      21.05
 C      -1.025829    -1.188697    -0.643200      57.15
 H      -0.639662    -2.085971    -0.771684      21.76
 C      -2.873437     0.342738    -0.668693      39.71
 H      -3.773025     0.664588    -0.957947      24.01
 C      -2.030409     1.299977    -0.102311     -10.30
 O      -2.666520     2.562729    -0.046244     182.53
 C      -3.752541     2.474319     1.087989      98.61
 H      -4.674602     2.614500     0.557761      25.97
 H      -3.827348     1.684493     1.824428      26.55
 H      -3.325762     3.356488     1.671274      23.55
 C      -0.521134     1.277735    -0.121577      12.10
 O       0.060416     2.398808     0.646127     193.03
 C      -0.155246    -0.041035    -0.230581      19.94
 H       1.070697    -0.147413     0.104734      17.23
 C      -2.320048    -0.991348    -0.805463      25.08
 C      -3.194016    -2.118146    -1.321716      82.70
 H      -4.047799    -1.668063    -1.879806      21.61
 O      -2.512478    -2.929121    -2.303588     246.66
 H      -2.920766    -3.838043    -2.239987      18.52
 C      -3.708379    -3.274402    -0.129513      75.57
 H      -2.739103    -3.849992    -0.049704      18.46
 O      -4.232539    -2.807300     1.104132     289.79
 H      -3.398112    -2.602754     1.779919      20.49
 C      -4.711545    -4.400715    -0.582705      96.36
 O      -3.931474    -5.395607    -1.671331     290.86
 H      -4.702896    -5.634612    -2.270803      33.87
 H      -5.560076    -4.171164    -1.081642      27.08
 H      -4.662387    -5.153595     0.270670      24.76
55
name = lig-etoh-frame_195
 C       2.963228     1.355411    -2.189923      14.95
 H       2.591657     2.124468    -2.827302      18.85
 C       3.740049     0.672751     0.184451      56.43
 H       3.918705     1.000191     1.288317      19.87
 C       4.379935    -0.312145    -0.397682      20.66
 O       5.043695    -1.382883     0.385411     211.71
 C       5.226362    -1.318968     1.821071     123.49
 H       4.388452    -1.856939     2.183929      26.62
 H       5.184719    -0.298094     2.291614      25.63
 H       6.294244    -1.701006     2.056360      26.46
 C       4.448686    -0.573611    -1.857733      16.10
 O       5.259864    -1.509553    -2.466104     204.24
 H       5.629889    -2.411617    -2.047977      21.57
 C       3.690832     0.303612    -2.701240      53.15
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 H       3.731815     0.219782    -3.855520      23.16
 C       2.880359     1.584735    -0.766126      65.25
 C       2.399075     2.982892    -0.184943     106.80
 H       2.914559     3.966412    -0.702255      21.88
 O       2.647590     3.192163     1.224722     298.87
 H       3.586796     3.672088     1.335013      26.61
 C       0.862725     3.132193    -0.349825      74.31
 H       0.641455     2.600563    -1.279141      19.78
 C       0.353671     4.617755    -0.084383      96.18
 O       1.184667     5.671831    -0.777543     205.72
 H       0.854823     5.652541    -1.786778      26.37
 H       0.482492     4.684881     1.098019      24.10
 H      -0.600644     4.576418    -0.477501      24.64
 C      -0.939787    -1.071619    -0.648048      36.49
 H      -0.792858    -2.329715    -0.608893      18.44
 C      -2.748659     0.262590    -0.626194      36.50
 H      -3.713258     0.742103    -1.183523      22.04
 C      -2.002307     1.315451    -0.071530       8.91
 O      -2.659164     2.528451    -0.002758     208.15
 C      -3.698901     2.588252     1.100136      98.96
 H      -4.806185     2.727171     0.629052      24.64
 H      -3.736848     1.701340     1.819981      25.34
 H      -3.684864     3.440798     1.818168      25.23
 C      -0.565784     1.299135    -0.038141      24.89
 O       0.045779     2.293672     0.576403     233.39
 C      -0.100005    -0.027222    -0.213791      40.71
 H       0.690770    -0.318619     0.281354      21.09
 C      -2.343554    -0.941837    -0.816728      40.40
 C      -3.261850    -2.131718    -1.361743      65.56
 H      -4.306459    -1.856448    -1.750998      22.07
 O      -2.514264    -2.952595    -2.367458     206.35
 H      -3.000252    -3.939632    -2.336352      16.12
 C      -3.714388    -3.295494    -0.184008      81.98
 H      -2.682728    -3.630832    -0.002362      19.11
 O      -4.230333    -2.799680     1.074177     325.62
 H      -3.559620    -2.808269     1.672115      28.43
 C      -4.674745    -4.475969    -0.639461      88.49
 O      -3.992600    -5.299420    -1.643901     342.85
 H      -4.652026    -5.557917    -2.233469      36.42
 H      -5.809245    -4.082584    -1.007951      24.02
 H      -4.657206    -5.229851     0.122139      24.64
55
name = lig-etoh-frame_196
 C       2.885226     1.348494    -2.227046      65.18
 H       2.471998     2.160012    -2.862085      21.93
 C       3.641087     0.781497     0.156744      51.84
 H       3.768503     0.567658     1.222515      22.00
 C       4.353571    -0.397859    -0.448799      12.29
 O       5.034982    -1.424657     0.320964     167.46
 C       5.177193    -1.235162     1.895598     111.36
 H       4.346629    -1.923188     2.261757      25.97
 H       5.045796    -0.291873     2.459585      25.29
 H       6.153039    -1.812209     2.010054      26.55
 C       4.471705    -0.548005    -1.827094      24.50
 O       5.196218    -1.493679    -2.469599     218.83
 H       5.511914    -2.269156    -1.899626      23.63
 C       3.738526     0.353353    -2.717124      45.81
 H       3.609243     0.003953    -3.702507      21.72
 C       2.845078     1.571069    -0.719305      38.34
 C       2.423674     2.943895    -0.112607     109.52
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 H       2.916378     3.549976    -0.889324      21.98
 O       2.698601     3.164199     1.234793     341.53
 H       3.482796     3.665707     1.374998      29.90
 C       0.856965     3.108090    -0.321194      77.50
 H       0.624813     3.043658    -1.452237      19.36
 C       0.385528     4.642798    -0.134977     104.43
 O       1.145934     5.647005    -0.745771     279.86
 H       0.895051     5.700605    -1.635345      31.42
 H       0.207977     4.791116     0.927836      26.55
 H      -0.780843     4.488109    -0.366433      23.44
 C      -0.864951    -1.049170    -0.632422      42.05
 H      -0.515961    -1.959293    -0.491496      23.93
 C      -2.726317     0.311495    -0.598962      52.09
 H      -3.621464     0.531819    -1.059074      22.08
 C      -1.967321     1.359007    -0.085287      27.50
 O      -2.674557     2.526084     0.080092     255.91
 C      -3.669929     2.703366     1.113573     104.74
 H      -4.718595     2.697389     0.666601      25.61
 H      -3.551626     1.692638     1.563813      25.47
 H      -3.759785     3.611981     1.792891      24.75
 C      -0.696888     1.249203     0.067065      32.37
 O       0.079051     2.226731     0.529912     237.08
 C      -0.053401    -0.042244    -0.199985      41.90
 H       0.862708    -0.537726     0.474338      18.56
 C      -2.350609    -1.010773    -0.883161      30.16
 C      -3.338795    -2.180980    -1.378646      65.15
 H      -4.366459    -1.813884    -1.681203      23.11
 O      -2.537381    -2.980895    -2.417497     264.93
 H      -2.926836    -3.780858    -2.477582      24.72
 C      -3.688225    -3.297121    -0.236760      87.25
 H      -2.705034    -3.698499     0.059072      20.21
 O      -4.255421    -2.792441     1.016926     269.30
 H      -3.441766    -2.781046     1.760029      22.06
 C      -4.631915    -4.528743    -0.690750     100.46
 O      -4.044500    -5.199399    -1.628077     325.40
 H      -4.618045    -5.449913    -2.480655      32.62
 H      -5.559328    -4.148132    -0.788287      28.02
 H      -4.941186    -5.141781     0.323433      26.15
55
name = lig-etoh-frame_197
 C       2.830611     1.359028    -2.175897      59.04
 H       2.235720     1.987296    -2.831033      22.83
 C       3.566817     0.786725     0.085561      58.51
 H       3.374196     0.648174     1.150806      23.03
 C       4.329678    -0.466656    -0.461840      12.41
 O       5.022274    -1.427906     0.281480     151.18
 C       5.101855    -1.210641     1.926163     100.89
 H       4.404309    -1.904059     2.400702      26.32
 H       5.068223    -0.195373     2.351558      25.05
 H       6.032721    -1.728835     2.105215      27.40
 C       4.463840    -0.492658    -1.819317      27.62
 O       5.148036    -1.495493    -2.482992     230.37
 H       5.318564    -2.084402    -1.787404      25.91
 C       3.767328     0.376659    -2.707042      40.12
 H       3.633599    -0.124426    -3.730245      21.15
 C       2.852879     1.567680    -0.682503      43.31
 C       2.390800     2.872652    -0.099717     108.65
 H       2.935910     3.539772    -0.901883      20.52
 O       2.748363     3.128269     1.262922     301.95
 H       3.528554     3.799454     1.321029      25.89
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 C       0.871647     3.133669    -0.340078      80.63
 H       0.659844     3.168170    -1.380062      21.43
 C       0.346017     4.603729    -0.142123     106.66
 O       1.109171     5.638055    -0.686428     231.49
 H       0.953590     5.568082    -1.767657      27.03
 H       0.228273     5.013126     0.943723      24.56
 H      -0.646301     4.692646    -0.472269      25.83
 C      -0.860542    -1.095602    -0.624200      30.35
 H      -0.066494    -2.044445    -0.596362      17.60
 C      -2.772459     0.313648    -0.613175      41.87
 H      -3.923876     0.531973    -0.840501      18.86
 C      -2.058869     1.411581    -0.111774      16.44
 O      -2.678877     2.595863     0.149374     266.01
 C      -3.657561     2.758028     1.126900     103.94
 H      -4.694175     2.690399     0.551743      23.43
 H      -3.589821     1.829432     1.726504      26.38
 H      -3.414677     3.683242     1.663308      25.41
 C      -0.687095     1.139122     0.163258      10.86
 O       0.146465     2.215754     0.518568     206.85
 C      -0.024107    -0.063576    -0.141018      43.32
 H       0.913757    -0.243367     0.239014      20.38
 C      -2.300358    -1.070225    -0.945436      24.85
 C      -3.367081    -2.250240    -1.370492      64.56
 H      -4.266235    -1.690043    -1.797608      23.35
 O      -2.576526    -2.968169    -2.450661     229.41
 H      -3.024241    -3.940979    -2.601159      16.50
 C      -3.644239    -3.307745    -0.252508      99.11
 H      -2.713711    -3.887678    -0.009173      20.86
 O      -4.273157    -2.784628     0.959871     322.06
 H      -3.550139    -2.483705     1.576319      26.00
 C      -4.619577    -4.499559    -0.604849      88.54
 O      -4.060931    -5.170952    -1.691462     360.76
 H      -4.511642    -5.096985    -2.588753      32.97
 H      -5.716212    -3.976626    -0.931191      25.76
 H      -4.861679    -4.993491     0.293981      28.08
55
name = lig-etoh-frame_198
 C       2.825631     1.346806    -2.099287      41.76
 H       2.024704     1.764916    -2.747244      21.83
 C       3.562627     0.623575     0.063377      66.07
 H       3.091689     1.007788     1.063161      19.21
 C       4.276173    -0.449296    -0.420438      28.72
 O       5.003855    -1.413215     0.298425     176.35
 C       5.028547    -1.223142     1.902222      92.21
 H       4.240893    -1.769721     2.448069      25.65
 H       5.085412    -0.093291     2.006952      23.80
 H       6.145729    -1.537932     2.230734      25.30
 C       4.450039    -0.438703    -1.859109      16.32
 O       5.108682    -1.501300    -2.495133     164.92
 H       5.289310    -2.198735    -1.694775      20.83
 C       3.721783     0.409893    -2.677550      55.12
 H       3.751862     0.096223    -3.701909      22.91
 C       2.846072     1.593810    -0.741817      66.50
 C       2.338195     2.846995    -0.137186     125.94
 H       2.888980     3.751434    -0.562412      21.80
 O       2.802123     3.090888     1.296375     270.33
 H       3.456606     3.875897     1.161959      25.40
 C       0.886809     3.181628    -0.358910      67.55
 H       0.672586     2.812650    -1.461667      20.81
 C       0.276582     4.570209    -0.069679     102.04
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 O       1.089513     5.645655    -0.675232     227.24
 H       1.127934     5.403120    -1.606585      31.40
 H       0.372522     4.924161     0.977906      23.90
 H      -0.702243     4.743417    -0.695796      22.19
 C      -0.847238    -1.218155    -0.617650      39.79
 H      -0.289826    -2.014589    -1.130621      18.28
 C      -2.884465     0.255990    -0.666592      42.30
 H      -3.941772     0.439920    -0.493392      20.74
 C      -2.161377     1.408745    -0.133163     -20.99
 O      -2.637422     2.693418     0.176537     223.36
 C      -3.667318     2.767192     1.155870     108.14
 H      -4.692502     2.914873     0.600126      23.81
 H      -3.780466     2.145240     2.129023      24.67
 H      -3.234296     3.725889     1.546492      24.26
 C      -0.622342     1.097444     0.224741      -3.03
 O       0.208285     2.216897     0.539754     179.09
 C      -0.071802    -0.083729    -0.083794      27.72
 H       1.160416     0.000043    -0.015482      16.53
 C      -2.229350    -1.063824    -0.960110      10.37
 C      -3.309888    -2.304425    -1.369039      73.04
 H      -4.125716    -1.691848    -1.864540      21.75
 O      -2.640982    -2.956942    -2.477553     263.30
 H      -3.031809    -3.896127    -2.556352      17.30
 C      -3.620180    -3.339676    -0.234148     106.59
 H      -2.680742    -3.868406    -0.096842      21.84
 O      -4.280062    -2.760014     0.900073     332.90
 H      -3.638365    -2.202221     1.416194      27.13
 C      -4.666240    -4.363001    -0.549357      94.02
 O      -4.058402    -5.184954    -1.769174     349.50
 H      -4.497254    -4.796112    -2.592735      29.47
 H      -5.493737    -4.008412    -0.946996      28.31
 H      -4.636626    -5.192386     0.378165      24.49
55
name = lig-etoh-frame_199
 C       2.811929     1.337576    -2.080983      40.84
 H       1.985871     1.684046    -2.690181      22.31
 C       3.495119     0.530244     0.096732      66.98
 H       3.376220     0.894006     1.053205      22.89
 C       4.249994    -0.426206    -0.392065      25.04
 O       4.978117    -1.403522     0.358618     218.94
 C       5.003319    -1.209687     1.822020     125.62
 H       4.062134    -1.548205     2.359210      26.42
 H       4.912501    -0.151092     1.803249      26.35
 H       5.912955    -1.468353     2.191105      29.44
 C       4.439499    -0.429872    -1.885946      14.99
 O       5.075631    -1.508789    -2.483460     203.69
 H       5.334411    -2.265804    -1.927697      22.77
 C       3.657024     0.436118    -2.647497      77.90
 H       3.770435     0.448996    -3.765919      26.15
 C       2.871506     1.585227    -0.796518      59.38
 C       2.323113     2.910652    -0.146831     116.79
 H       2.836515     3.829694    -0.544847      21.68
 O       2.835183     3.044487     1.309163     295.41
 H       3.404824     3.783977     1.237493      28.07
 C       0.859044     3.171175    -0.394755      72.99
 H       0.663090     2.678017    -1.292903      22.96
 C       0.225248     4.569564    -0.029122     100.20
 O       1.085739     5.648591    -0.667773     227.82
 H       1.216866     5.349642    -1.610744      30.05
 H       0.239055     4.611671     1.087040      24.63
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 H      -0.763129     4.523157    -0.471257      24.50
 C      -0.844774    -1.303317    -0.643107      25.92
 H      -0.510597    -2.159044    -1.393879      17.24
 C      -2.959405     0.213907    -0.674794      41.41
 H      -4.075765     0.181955    -0.467661      21.84
 C      -2.177042     1.332844    -0.143734     -22.65
 O      -2.571723     2.737626     0.180795     177.16
 C      -3.688064     2.839787     1.222592     112.22
 H      -4.725055     3.076631     0.756966      24.86
 H      -3.789714     2.276817     2.120444      26.59
 H      -3.517244     3.850126     1.588991      26.70
 C      -0.645237     1.166561     0.231585     -16.51
 O       0.246662     2.202037     0.596779     166.64
 C      -0.090723    -0.159545    -0.046299      11.12
 H       0.916260    -0.031074    -0.388794      18.27
 C      -2.205649    -1.039349    -0.926842      11.44
 C      -3.189363    -2.299820    -1.384782      72.33
 H      -4.162836    -1.821024    -1.704616      21.46
 O      -2.699147    -2.956130    -2.508890     291.52
 H      -2.982506    -3.878373    -2.433523      15.67
 C      -3.605172    -3.339208    -0.215500      99.29
 H      -2.595426    -3.811476     0.021650      20.66
 O      -4.271458    -2.719107     0.860994     308.39
 H      -3.687885    -1.885965     1.283765      22.66
 C      -4.643459    -4.317529    -0.542638      90.14
 O      -4.066142    -5.195795    -1.795950     351.71
 H      -4.518785    -4.709931    -2.640267      26.57
 H      -5.776737    -3.884513    -0.877573      24.72
 H      -4.645764    -5.043116     0.111766      26.78
55
name = lig-etoh-frame_200
 C       2.757263     1.350746    -2.131171      46.79
 H       2.064791     1.913880    -2.782417      21.79
 C       3.375740     0.575103     0.139736      55.62
 H       3.695344     0.620427     1.306918      20.33
 C       4.281354    -0.460419    -0.424841      24.47
 O       4.945495    -1.408734     0.401136     238.52
 C       4.937420    -1.146123     1.709114     120.79
 H       4.039830    -1.510367     2.195377      26.88
 H       4.851523    -0.014074     1.967358      23.49
 H       5.913048    -1.663270     2.284651      24.80
 C       4.417371    -0.476760    -1.855624      21.11
 O       5.054122    -1.506239    -2.495343     230.61
 H       5.329684    -2.250361    -1.987434      24.81
 C       3.635842     0.413918    -2.671490      55.15
 H       3.730028     0.648704    -3.740968      22.64
 C       2.901193     1.572620    -0.713770      38.43
 C       2.367233     2.994031    -0.129537      89.74
 H       2.862696     3.801764    -0.841028      21.45
 O       2.827508     2.980795     1.291955     285.88
 H       3.539760     3.773958     1.449513      23.61
 C       0.808135     3.119627    -0.374423      66.94
 H       0.506514     2.784192    -1.454461      18.51
 C       0.221271     4.552828    -0.030471      90.04
 O       1.064818     5.635142    -0.636175     207.55
 H       1.125654     5.354851    -1.678805      26.59
 H       0.097144     4.421570     1.115734      23.24
 H      -0.924190     4.466652    -0.213121      22.29
 C      -0.864673    -1.303747    -0.683140      18.12
 H      -0.527437    -2.285816    -1.216952      18.10
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 C      -2.967335     0.185070    -0.624757      32.12
 H      -4.083910    -0.032616    -0.737353      18.90
 C      -2.127630     1.274783    -0.113233       0.98
 O      -2.533653     2.724025     0.196146     153.72
 C      -3.700170     2.981708     1.267841      79.40
 H      -4.812799     2.914823     0.760223      23.38
 H      -3.606222     2.061439     1.999002      22.72
 H      -3.719309     4.021800     1.718301      24.56
 C      -0.729095     1.196572     0.179401      -1.66
 O       0.247633     2.164682     0.670245     160.49
 C      -0.134394    -0.229873    -0.074829      12.43
 H       0.966379    -0.263882    -0.444030      18.79
 C      -2.258298    -1.045387    -0.875494      15.30
 C      -3.096632    -2.234933    -1.376745      70.85
 H      -4.189871    -1.912555    -1.434057      20.29
 O      -2.730395    -2.965459    -2.562937     271.80
 H      -2.857124    -4.028935    -2.258356      12.77
 C      -3.541180    -3.287967    -0.202268     100.49
 H      -2.711193    -3.810781     0.258514      22.82
 O      -4.255625    -2.635173     0.850303     364.31
 H      -3.749090    -1.952258     1.144825      30.56
 C      -4.630724    -4.325480    -0.655119      89.14
 O      -4.096460    -5.174104    -1.774462     379.73
 H      -4.468787    -5.020377    -2.638016      34.77
 H      -5.542159    -3.890683    -0.613902      28.50
 H      -4.821448    -5.183427     0.268052      24.52
55
name = lig-etoh-frame_201
 C       2.722476     1.368531    -2.147462      43.74
 H       2.343465     2.203185    -2.787641      23.07
 C       3.345324     0.600506     0.189105      58.43
 H       3.556940     0.628497     1.203749      23.31
 C       4.268579    -0.464124    -0.469077      23.22
 O       4.915172    -1.416875     0.360141     234.45
 C       4.885565    -1.067872     1.714778     133.63
 H       3.957697    -1.607166     2.126552      25.35
 H       5.086499    -0.105284     2.121951      26.98
 H       5.592838    -1.642749     2.116565      29.67
 C       4.371621    -0.547382    -1.809793      22.84
 O       5.050253    -1.502170    -2.538669     195.25
 H       5.322180    -2.276191    -1.840351      22.78
 C       3.617171     0.396450    -2.705268      36.80
 H       3.795424     0.399526    -3.790812      21.56
 C       2.870035     1.604223    -0.614532      21.03
 C       2.435920     3.025402    -0.132544      90.01
 H       2.897755     3.715080    -0.816084      21.89
 O       2.805751     2.946811     1.254369     331.57
 H       3.498551     3.576907     1.505981      27.32
 C       0.759466     3.065705    -0.324850      75.47
 H       0.464474     2.958863    -1.341437      19.99
 C       0.213459     4.491860    -0.025839     100.42
 O       1.015810     5.598104    -0.598970     251.95
 H       0.896259     5.456894    -1.509807      32.97
 H       0.313808     4.644758     1.057030      25.37
 H      -0.862469     4.671618    -0.234238      24.67
 C      -0.918004    -1.244008    -0.703857      39.17
 H      -0.379570    -2.255693    -0.890145      21.48
 C      -2.917235     0.141129    -0.557313      42.10
 H      -3.942385     0.190733    -0.907314      21.25
 C      -2.101846     1.291705    -0.038682       9.17
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 O      -2.532020     2.692591     0.220355     186.80
 C      -3.703338     3.057706     1.279587      94.26
 H      -4.665452     2.784063     0.736639      24.85
 H      -3.485002     2.226141     1.830613      25.87
 H      -3.618197     4.002357     1.753885      26.06
 C      -0.762559     1.115489     0.107331      23.68
 O       0.202321     2.108855     0.717039     176.66
 C      -0.172580    -0.250395    -0.171934      23.77
 H       0.960784    -0.483663     0.010602      19.20
 C      -2.326467    -1.077856    -0.837045      33.22
 C      -3.089036    -2.192516    -1.325602      67.95
 H      -4.088784    -1.777814    -1.485866      21.45
 O      -2.738165    -2.990332    -2.603733     311.39
 H      -2.758149    -3.836519    -2.321989      23.18
 C      -3.472301    -3.245348    -0.182372      87.40
 H      -2.718152    -3.853317     0.404614      19.89
 O      -4.255492    -2.545406     0.835978     294.56
 H      -3.577727    -1.872907     1.283636      22.06
 C      -4.574133    -4.398950    -0.730114      86.24
 O      -4.129413    -5.150989    -1.725261     346.63
 H      -4.545688    -5.213389    -2.685526      29.98
 H      -5.622765    -3.716432    -0.770513      26.44
 H      -4.755373    -4.922565     0.083081      28.16
55
name = lig-etoh-frame_202
 C       2.764865     1.385884    -2.108214      76.03
 H       2.592770     2.291962    -2.661947      26.72
 C       3.392848     0.580430     0.179976      50.53
 H       3.293315     0.843649     1.336382      19.55
 C       4.191149    -0.430932    -0.449764      19.67
 O       4.887791    -1.401953     0.274415     178.77
 C       4.815093    -1.047715     1.780304      99.64
 H       3.872868    -1.359988     2.171375      25.67
 H       5.269032    -0.024138     2.090437      24.71
 H       5.673101    -1.878349     2.147520      24.33
 C       4.285890    -0.585392    -1.852765      14.01
 O       5.064223    -1.519983    -2.566217     222.88
 H       5.313413    -2.195967    -1.937612      26.12
 C       3.583850     0.387786    -2.698938      42.47
 H       3.814562    -0.002761    -3.740057      20.47
 C       2.798038     1.642137    -0.616384      20.98
 C       2.452993     2.964340    -0.132588      98.12
 H       3.023878     3.900459    -0.686176      19.73
 O       2.768058     2.935760     1.228413     325.76
 H       3.503067     3.575800     1.387183      27.26
 C       0.742635     3.044707    -0.235661      56.12
 H       0.469508     2.754443    -1.310526      20.54
 C       0.215589     4.453424     0.029942      99.59
 O       0.958766     5.551853    -0.558648     182.18
 H       0.714540     5.574808    -1.608013      26.93
 H       0.547488     4.892321     1.054098      21.95
 H      -0.800759     4.706077    -0.356600      23.02
 C      -0.979006    -1.209164    -0.720431      48.16
 H      -0.349333    -2.184032    -0.472607      19.68
 C      -2.859121     0.149176    -0.480538      48.36
 H      -3.824659     0.651558    -0.932024      20.38
 C      -2.136919     1.337171     0.042607      -9.45
 O      -2.545338     2.659193     0.238254     200.47
 C      -3.657619     3.049814     1.241412      82.61
 H      -4.727178     2.805548     0.620741      22.55
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 H      -3.496239     2.311000     2.178470      23.43
 H      -3.436815     4.056093     1.634829      24.60
 C      -0.696166     0.996714     0.064137       8.80
 O       0.125905     2.039613     0.716103     175.29
 C      -0.178308    -0.201319    -0.246612      43.79
 H       0.734459    -0.433648     0.325753      19.36
 C      -2.330000    -1.103746    -0.818099      34.49
 C      -3.163349    -2.229247    -1.284356      67.01
 H      -4.074864    -1.675957    -1.741156      20.90
 O      -2.728276    -2.964988    -2.618703     248.48
 H      -2.727175    -3.994147    -2.354607      18.39
 C      -3.452628    -3.230695    -0.160418     101.71
 H      -2.605899    -3.714390     0.279879      22.80
 O      -4.244118    -2.439121     0.813293     300.04
 H      -3.535063    -2.119462     1.572450      21.84
 C      -4.552962    -4.341613    -0.738408      89.50
 O      -4.131937    -5.189519    -1.726494     329.56
 H      -4.713893    -5.024407    -2.543174      29.44
 H      -5.316698    -3.828733    -1.212090      26.94
 H      -4.719738    -5.003893     0.318125      24.35
55
name = lig-etoh-frame_203
 C       2.859457     1.426672    -2.034209      68.94
 H       2.617531     2.314865    -2.666588      24.78
 C       3.435285     0.606666     0.153033      79.06
 H       3.124215     0.869147     1.180977      20.70
 C       4.100252    -0.409533    -0.422656      20.03
 O       4.855292    -1.363709     0.232544     141.37
 C       4.822838    -1.094365     1.832085     101.76
 H       3.741407    -0.989675     2.268071      24.68
 H       5.207961    -0.112131     1.876962      26.84
 H       5.404656    -1.816735     2.185869      28.62
 C       4.176443    -0.580801    -1.927222      21.73
 O       5.071072    -1.528948    -2.577789     215.52
 H       5.362625    -2.260735    -2.019964      25.91
 C       3.561002     0.327121    -2.663324      63.83
 H       3.573373     0.027924    -3.693574      22.20
 C       2.772712     1.586307    -0.724491      56.99
 C       2.398860     2.913061    -0.125641     124.67
 H       2.847877     3.760025    -0.517518      24.39
 O       2.734943     2.950101     1.245483     312.93
 H       3.532355     3.648752     1.252916      25.27
 C       0.752414     3.017925    -0.169044      59.95
 H       0.531419     2.552818    -1.120590      22.23
 C       0.234716     4.467833     0.123292     106.28
 O       0.916576     5.523951    -0.565757     273.24
 H       0.728300     5.528717    -1.534882      29.51
 H       0.310247     4.659547     1.162108      26.23
 H      -0.877668     4.430188    -0.215535      23.22
 C      -0.976169    -1.238527    -0.691450      47.76
 H      -0.634772    -2.215844    -0.499736      23.37
 C      -2.847410     0.270008    -0.421110      50.68
 H      -3.758964     0.617415    -0.761500      22.80
 C      -2.122193     1.308670     0.095168       3.22
 O      -2.568382     2.623995     0.261702     245.40
 C      -3.585503     2.968240     1.203847     127.67
 H      -4.621321     2.976301     0.751765      26.39
 H      -3.698337     2.618914     2.191240      27.42
 H      -3.395110     4.060101     1.241912      26.12
 C      -0.673351     1.021278     0.077588      17.64
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 O       0.059707     1.974147     0.694248     199.69
 C      -0.152464    -0.156128    -0.302818      46.33
 H       0.735427    -0.377993     0.485274      19.11
 C      -2.330322    -1.103615    -0.819530      14.60
 C      -3.265337    -2.274621    -1.312191      75.51
 H      -4.135966    -1.850021    -1.705126      24.52
 O      -2.708418    -2.932538    -2.589206     274.38
 H      -2.764721    -3.974897    -2.506047      18.20
 C      -3.513822    -3.214305    -0.169597     101.35
 H      -2.477130    -3.519528     0.150860      23.42
 O      -4.206028    -2.349615     0.811629     313.86
 H      -3.700607    -2.375626     1.617544      28.30
 C      -4.515489    -4.257775    -0.647268      98.72
 O      -4.109661    -5.267370    -1.760260     317.66
 H      -4.631817    -4.926025    -2.444726      31.84
 H      -5.340247    -3.708940    -1.298406      25.28
 H      -4.875062    -4.825659     0.106070      27.86
55
name = lig-etoh-frame_204
 C       2.967591     1.476288    -2.073709      52.61
 H       2.517878     2.200666    -2.723757      20.43
 C       3.415506     0.682552     0.107619      73.99
 H       3.241477     0.738185     1.184563      21.63
 C       4.049184    -0.441320    -0.450196      12.58
 O       4.815360    -1.330498     0.255759     163.38
 C       4.800826    -1.121449     1.811760      96.84
 H       3.841240    -0.850829     2.195261      26.18
 H       5.337687    -0.098750     1.799915      24.94
 H       5.344948    -2.035094     2.414029      24.87
 C       4.131812    -0.630525    -1.915717      23.46
 O       5.054144    -1.513469    -2.580423     171.12
 H       5.323046    -2.368244    -1.983404      22.68
 C       3.493814     0.295822    -2.672843      65.54
 H       3.285771     0.354144    -3.786442      24.68
 C       2.799018     1.517594    -0.764757      59.41
 C       2.261410     2.836247    -0.087549     122.10
 H       2.675048     3.813943    -0.755362      22.66
 O       2.723637     2.986913     1.290526     318.95
 H       3.456419     3.569926     1.338687      29.89
 C       0.790381     2.974499    -0.128014      66.89
 H       0.501206     2.680331    -1.174586      21.72
 C       0.219010     4.451201     0.198626     105.75
 O       0.886572     5.508460    -0.568054     259.57
 H       0.725582     5.268175    -1.525329      29.17
 H       0.057238     4.429952     1.365868      24.36
 H      -0.841902     4.267237     0.045032      24.73
 C      -0.953820    -1.279176    -0.637100      14.90
 H      -0.767619    -2.509762    -0.796393      20.40
 C      -2.875106     0.333890    -0.414255      39.33
 H      -4.058830     0.398249    -0.555809      22.89
 C      -2.048815     1.257843     0.117596      32.33
 O      -2.574151     2.565039     0.285833     245.14
 C      -3.532069     2.941280     1.153132     125.18
 H      -4.734794     2.994333     0.783864      24.34
 H      -3.651190     2.657504     2.276144      25.10
 H      -3.414503     4.038017     1.009579      25.50
 C      -0.726855     1.120800     0.108443      21.18
 O       0.047243     1.960674     0.705839     205.25
 C      -0.100608    -0.169840    -0.308950      31.60
 H       0.832886    -0.292614     0.077300      22.15
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 C      -2.376596    -1.038473    -0.829992     -11.23
 C      -3.318608    -2.273348    -1.385736      63.67
 H      -4.456812    -1.929343    -1.585626      23.93
 O      -2.688472    -2.900202    -2.535681     292.79
 H      -2.858715    -3.802952    -2.533380      21.63
 C      -3.571583    -3.178176    -0.185771     112.53
 H      -2.590417    -3.469955     0.153025      26.47
 O      -4.166284    -2.280092     0.803332     238.51
 H      -3.769809    -2.601978     1.793328      24.57
 C      -4.505569    -4.200851    -0.614198      86.81
 O      -4.072784    -5.331340    -1.755850     241.31
 H      -4.521273    -4.940313    -2.681227      25.11
 H      -5.356790    -3.567348    -0.898138      26.78
 H      -5.164578    -4.825876     0.197017      26.16
55
name = lig-etoh-frame_205
 C       3.049179     1.499921    -2.203003      47.55
 H       2.407135     2.171227    -2.824867      21.19
 C       3.400259     0.682041     0.077443      46.50
 H       3.477287     0.678294     1.250256      20.23
 C       4.028800    -0.486597    -0.509237      17.50
 O       4.776209    -1.329162     0.328248     230.93
 C       4.815701    -1.116737     1.744214     126.72
 H       3.763826    -0.940368     2.127858      25.17
 H       5.550936    -0.360924     2.004909      27.87
 H       5.104312    -1.962146     2.312174      28.51
 C       4.134732    -0.713213    -1.869323      23.28
 O       5.020491    -1.503288    -2.562291     230.86
 H       5.149759    -2.264692    -2.033619      26.85
 C       3.395852     0.319616    -2.741406      47.65
 H       3.284886     0.408537    -3.810942      24.97
 C       2.812300     1.565354    -0.713230      53.29
 C       2.176018     2.785295    -0.059572     131.12
 H       2.399516     3.506397    -0.747470      26.42
 O       2.694063     3.014694     1.332941     261.79
 H       3.555960     3.623283     1.364008      25.73
 C       0.774833     2.945446    -0.119702      82.74
 H       0.454097     2.981076    -1.187201      21.61
 C       0.187886     4.373033     0.287517      89.46
 O       0.839981     5.482937    -0.551619     215.64
 H       0.764001     4.981058    -1.483349      27.43
 H       0.290841     4.576943     1.324787      25.41
 H      -0.958548     4.322865    -0.022399      22.56
 C      -0.973258    -1.326810    -0.607931      33.63
 H      -0.627538    -2.201869    -0.982519      21.70
 C      -2.966829     0.250196    -0.466183      60.11
 H      -3.977228     0.339364    -0.238203      27.23
 C      -2.065243     1.255106     0.119615      20.79
 O      -2.537292     2.487341     0.290916     232.42
 C      -3.565341     2.985397     1.138333     115.74
 H      -4.669045     2.689010     0.712776      24.38
 H      -3.317544     2.590723     2.114812      26.05
 H      -3.453486     4.075161     1.138014      26.21
 C      -0.712950     1.094929     0.103409      21.17
 O       0.098667     2.022347     0.760736     201.19
 C      -0.110081    -0.198137    -0.282399      13.48
 H       1.158896    -0.218945    -0.523148      20.13
 C      -2.426494    -0.938830    -0.840219      -3.17
 C      -3.362750    -2.193947    -1.440199      80.25
 H      -4.337383    -1.898418    -1.628627      26.40
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 O      -2.667420    -2.850154    -2.475733     242.38
 H      -3.058477    -3.884735    -2.485658      16.89
 C      -3.567462    -3.120702    -0.187759     106.56
 H      -2.666956    -3.627563     0.260957      25.84
 O      -4.132682    -2.240922     0.809250     303.13
 H      -3.852530    -2.535972     1.652338      29.21
 C      -4.584006    -4.234672    -0.595222      73.87
 O      -4.052569    -5.335473    -1.729762     280.05
 H      -4.345077    -5.190187    -2.626536      29.23
 H      -5.481473    -3.531586    -0.868590      26.32
 H      -4.951464    -4.820922     0.220391      28.29
55
name = lig-etoh-frame_206
 C       3.037490     1.547431    -2.256086      38.42
 H       2.461139     2.222898    -2.884590      21.25
 C       3.422548     0.591798     0.075166      43.25
 H       3.522702     0.812571     1.057756      22.79
 C       4.029419    -0.519410    -0.527805      17.44
 O       4.751545    -1.358418     0.387557     230.14
 C       4.809960    -1.092733     1.689518     127.61
 H       3.799651    -0.930932     2.111103      25.51
 H       5.638857    -0.497342     2.207634      26.68
 H       5.043023    -2.202489     2.131464      25.13
 C       4.095895    -0.718682    -1.895031      19.79
 O       4.980747    -1.507800    -2.540115     212.08
 H       5.123387    -2.365058    -2.052313      24.73
 C       3.360051     0.298144    -2.801139      41.10
 H       3.465406     0.073150    -3.912331      23.52
 C       2.828537     1.672371    -0.710082      25.69
 C       2.191819     2.756388    -0.018410     111.55
 H       2.498325     3.685672    -0.824626      21.45
 O       2.656555     3.045152     1.355998     289.37
 H       3.494805     3.578397     1.203046      26.60
 C       0.666531     2.966009    -0.104750      84.29
 H       0.372784     2.918096    -1.167959      22.09
 C       0.158530     4.313894     0.341916     102.96
 O       0.776783     5.416850    -0.527579     234.93
 H       0.862295     5.121086    -1.416758      32.23
 H       0.597854     4.767257     1.311668      23.57
 H      -0.829109     4.403211     0.044722      25.40
 C      -1.033135    -1.267420    -0.601928      33.78
 H      -0.363799    -2.100237    -1.249360      20.34
 C      -3.031359     0.191306    -0.474972      52.53
 H      -4.108914     0.357375    -0.126016      22.66
 C      -2.150214     1.209156     0.080228      -1.95
 O      -2.490118     2.468459     0.283585     197.88
 C      -3.608373     3.019327     1.134845     105.99
 H      -4.463947     2.291561     0.795884      23.71
 H      -3.229415     2.553226     2.075875      25.38
 H      -3.579046     4.094797     1.244123      25.72
 C      -0.633663     0.993215     0.112211     -10.05
 O       0.143823     2.079909     0.813499     191.69
 C      -0.116356    -0.237744    -0.278744      45.98
 H       0.714279    -0.222756    -0.776994      24.73
 C      -2.439090    -0.953856    -0.877038      20.57
 C      -3.341281    -2.076823    -1.410711      72.39
 H      -4.373563    -1.651657    -1.909360      22.27
 O      -2.654740    -2.826306    -2.431729     265.94
 H      -3.059188    -3.684508    -2.414959      23.76
 C      -3.548820    -3.084813    -0.192108      89.32
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 H      -2.707619    -3.667339     0.186536      24.09
 O      -4.122509    -2.215239     0.800392     303.51
 H      -3.761533    -2.404640     1.707908      27.22
 C      -4.672253    -4.271951    -0.611382      74.59
 O      -4.035901    -5.303001    -1.660290     303.10
 H      -4.475078    -5.256557    -2.563463      29.93
 H      -5.600527    -3.856961    -1.100565      25.63
 H      -4.723742    -5.009851     0.338100      25.32
55
name = lig-etoh-frame_207
 C       2.954128     1.581522    -2.233648      46.41
 H       2.608342     2.382918    -2.917630      20.89
 C       3.413627     0.554112     0.016830      53.45
 H       3.521060     0.938385     1.152950      20.21
 C       4.047669    -0.541549    -0.491695       9.98
 O       4.740548    -1.400708     0.349742     206.99
 C       4.803411    -1.130272     1.752211     126.89
 H       3.860324    -0.761313     2.196710      25.20
 H       5.597768    -0.463765     2.120370      27.77
 H       4.973316    -2.168538     1.948581      26.45
 C       4.013965    -0.655212    -1.966972      18.94
 O       4.948362    -1.541265    -2.527768     175.84
 H       5.151981    -2.492504    -2.096050      22.61
 C       3.393108     0.239214    -2.821891      57.41
 H       3.591998    -0.177037    -3.815478      22.35
 C       2.902993     1.679952    -0.769950      35.65
 C       2.236619     2.856129    -0.023762     134.32
 H       2.617473     3.708824    -0.466446      25.27
 O       2.615200     3.069037     1.346750     332.90
 H       3.442599     3.546403     1.227195      28.98
 C       0.590922     3.006114    -0.094607      77.64
 H       0.237232     2.624413    -1.096389      22.47
 C       0.186104     4.337470     0.356424      99.25
 O       0.717637     5.355418    -0.496730     286.00
 H       0.847800     5.223350    -1.514665      27.03
 H       0.611408     4.605515     1.330139      24.95
 H      -1.041121     4.425244     0.413416      22.96
 C      -1.085879    -1.198348    -0.675877      68.61
 H      -0.679150    -1.936922    -1.163086      23.25
 C      -3.079461     0.215779    -0.413998      38.34
 H      -4.193739     0.260301    -0.409386      20.27
 C      -2.170129     1.124509     0.025225       0.43
 O      -2.448096     2.521657     0.271441     197.48
 C      -3.605313     2.949824     1.151049     109.04
 H      -4.546662     2.357887     0.926298      25.63
 H      -3.409222     2.690142     2.230550      25.97
 H      -3.826729     4.071039     1.074230      25.78
 C      -0.624847     0.931806     0.178709      -6.06
 O       0.131552     2.056773     0.854972     184.22
 C      -0.165781    -0.259894    -0.277026      48.56
 H       0.911246    -0.377714    -0.933555      20.38
 C      -2.416159    -1.053510    -0.914669      26.44
 C      -3.312154    -1.987977    -1.374310      99.53
 H      -4.092582    -1.543277    -1.844093      25.15
 O      -2.636382    -2.797257    -2.402878     264.56
 H      -3.037177    -3.715525    -2.378561      21.49
 C      -3.605199    -3.056576    -0.222644      62.57
 H      -2.620694    -3.556917    -0.014224      24.28
 O      -4.131839    -2.210213     0.802146     310.04
 H      -3.482685    -2.128538     1.718836      22.18
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 C      -4.707229    -4.336012    -0.642752      92.39
 O      -4.022552    -5.242324    -1.581735     312.51
 H      -4.769410    -5.233589    -2.338825      28.38
 H      -5.707096    -4.182639    -1.100985      25.19
 H      -4.655142    -4.956572     0.287802      25.56
55
name = lig-etoh-frame_208
 C       2.865156     1.551608    -2.202436      92.05
 H       2.754647     2.463069    -2.812415      27.33
 C       3.388793     0.607522    -0.014203      74.72
 H       3.439117     0.781613     0.977506      25.53
 C       4.053929    -0.536870    -0.481486       7.80
 O       4.734376    -1.445048     0.263576     166.11
 C       4.791269    -1.185943     1.831833      97.88
 H       3.874367    -0.653648     2.252307      23.92
 H       5.628741    -0.426536     1.901094      25.81
 H       4.998831    -2.213630     2.266171      25.22
 C       3.979970    -0.642459    -1.964633      25.04
 O       4.917540    -1.590162    -2.535896     219.33
 H       4.991139    -2.382962    -2.078858      27.72
 C       3.428676     0.238339    -2.806228      49.21
 H       3.546386    -0.034035    -3.867719      20.93
 C       2.973041     1.642731    -0.861444      27.66
 C       2.263341     2.982261    -0.062875     100.13
 H       2.774257     4.048583    -0.439047      19.58
 O       2.575836     3.074768     1.334249     288.72
 H       3.503397     3.588403     1.486396      25.18
 C       0.586466     2.990086    -0.102450      57.09
 H       0.169721     2.632032    -1.018126      23.79
 C       0.164099     4.401741     0.359989     114.29
 O       0.676743     5.337784    -0.478755     322.08
 H       0.556416     5.048585    -1.478036      26.92
 H       0.594610     4.377174     1.436378      24.40
 H      -0.807758     4.385472     0.715064      27.13
 C      -1.122941    -1.162554    -0.794462      56.15
 H      -0.813639    -2.300305    -1.239681      19.37
 C      -3.088582     0.185746    -0.378199      49.70
 H      -4.127973     0.305083    -0.687176      17.70
 C      -2.122496     1.124887     0.019229       0.33
 O      -2.434178     2.579221     0.271889     183.08
 C      -3.589588     2.853480     1.171975     114.90
 H      -4.728416     2.481174     0.961544      24.99
 H      -3.493472     2.874078     2.268879      27.23
 H      -3.891175     3.829461     0.795481      27.14
 C      -0.690913     0.935743     0.283030       0.30
 O       0.074996     1.959940     0.887115     187.35
 C      -0.141165    -0.255841    -0.315564      42.13
 H       0.831984    -0.499714    -0.403037      21.65
 C      -2.420488    -1.013848    -0.864756      32.35
 C      -3.298389    -2.038479    -1.382950      83.86
 H      -4.250819    -1.385125    -1.793245      23.24
 O      -2.617955    -2.775157    -2.392260     221.31
 H      -2.970593    -3.797242    -2.360738      20.02
 C      -3.716789    -3.019071    -0.276024      72.43
 H      -2.692989    -3.425372    -0.163923      24.49
 O      -4.135901    -2.217489     0.844796     352.66
 H      -3.417108    -1.998094     1.360987      30.57
 C      -4.673167    -4.374559    -0.645363      91.91
 O      -4.029746    -5.173475    -1.535409     346.19
 H      -4.684687    -5.358512    -2.150709      33.09
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 H      -5.844189    -4.270914    -0.829444      24.13
 H      -4.819753    -4.880773     0.409637      24.51
55
name = lig-etoh-frame_209
 C       2.825372     1.459704    -2.242135      78.05
 H       2.704702     2.402237    -2.756192      26.57
 C       3.389684     0.648949    -0.034071      65.14
 H       3.293169     0.769783     1.128155      22.28
 C       4.023347    -0.491089    -0.521010      17.77
 O       4.725960    -1.502636     0.212924     153.08
 C       4.789724    -1.229024     1.859486      99.58
 H       3.907405    -0.787346     2.192444      26.18
 H       5.653771    -0.553757     1.758634      26.14
 H       5.028121    -2.060895     2.617271      25.99
 C       4.032053    -0.712440    -1.902688      24.87
 O       4.867370    -1.621866    -2.556864     214.69
 H       4.822682    -2.430357    -1.935361      25.67
 C       3.422333     0.327215    -2.790968      49.15
 H       3.414868     0.327527    -3.916986      20.40
 C       2.977319     1.672664    -0.881200      30.96
 C       2.306563     3.106322    -0.127922      90.96
 H       2.582514     3.936875    -0.630394      22.81
 O       2.552909     3.070780     1.333274     338.64
 H       3.350252     3.534464     1.544929      29.54
 C       0.624918     2.952933    -0.097364      32.00
 H       0.184149     2.797456    -1.146462      21.68
 C       0.150691     4.394912     0.428081      92.36
 O       0.637565     5.364082    -0.490594     285.08
 H       0.360259     4.992606    -1.305621      31.53
 H       0.801720     4.381463     1.340849      23.92
 H      -1.034885     4.461691     0.739358      23.44
 C      -1.045975    -1.200266    -0.933866      40.54
 H      -0.858882    -2.189354    -1.095084      24.25
 C      -3.040654     0.161941    -0.365735      60.35
 H      -4.032057     0.552092    -0.820436      20.28
 C      -2.079295     1.214742     0.066900      -0.72
 O      -2.452525     2.588313     0.289443     196.77
 C      -3.611209     2.795258     1.153471     114.10
 H      -4.529251     2.197648     0.939624      26.02
 H      -3.343702     2.965642     2.257241      25.93
 H      -3.789183     3.809063     0.701211      25.65
 C      -0.763952     0.922207     0.348500      13.32
 O       0.020035     1.855450     0.909810     154.14
 C      -0.155325    -0.234033    -0.328423       5.86
 H       0.993320    -0.547440     0.128669      18.07
 C      -2.498559    -0.913324    -0.787698      21.52
 C      -3.367536    -2.101978    -1.437470     101.25
 H      -4.213397    -1.629123    -1.767251      27.45
 O      -2.606947    -2.781459    -2.402725     284.72
 H      -2.855001    -3.645639    -2.378517      25.03
 C      -3.831662    -2.999470    -0.326700      95.22
 H      -2.874420    -3.527542    -0.046757      22.42
 O      -4.170358    -2.250185     0.878197     266.53
 H      -3.184304    -1.900111     1.228229      22.05
 C      -4.667302    -4.339776    -0.538425     102.00
 O      -4.018674    -5.128255    -1.527885     328.46
 H      -4.585387    -5.584750    -2.222593      31.33
 H      -5.703007    -4.082700    -0.771900      25.67
 H      -4.799086    -4.788397     0.498035      26.24
55
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name = lig-etoh-frame_210
 C       2.816927     1.413218    -2.273998      75.28
 H       2.434451     2.228021    -2.958740      26.15
 C       3.401093     0.697416    -0.002810      60.77
 H       3.180911     0.850371     1.035231      21.27
 C       4.001427    -0.475342    -0.552402      19.92
 O       4.702731    -1.563132     0.213413     158.36
 C       4.816127    -1.261293     1.827407     100.55
 H       3.763360    -0.813169     2.113051      24.05
 H       5.652053    -0.567595     1.874774      27.05
 H       5.039572    -2.060129     2.509469      27.32
 C       4.083125    -0.723863    -1.920868      28.27
 O       4.799460    -1.665730    -2.561384     214.90
 H       4.867840    -2.532038    -1.956329      24.87
 C       3.429450     0.374106    -2.775477      67.95
 H       3.414025     0.429056    -3.834508      19.84
 C       2.920886     1.763400    -0.826499      40.50
 C       2.307343     3.093141    -0.164002      79.72
 H       2.451698     4.077552    -0.929064      16.82
 O       2.531795     3.069485     1.306911     303.37
 H       3.406876     3.584169     1.452052      26.30
 C       0.659471     2.942504    -0.093284      30.50
 H       0.306678     2.835574    -1.094109      21.77
 C       0.139801     4.336393     0.529395      92.59
 O       0.590474     5.405593    -0.494930     167.52
 H       0.249496     5.104891    -1.482703      26.01
 H       0.832027     4.632721     1.343882      24.21
 H      -0.858436     4.490307     0.545942      25.65
 C      -0.982142    -1.177263    -0.996337      22.87
 H      -0.621503    -2.323987    -1.153511      22.73
 C      -2.997742     0.313208    -0.342949      43.26
 H      -3.932762     0.637585    -0.636322      23.69
 C      -2.101861     1.311140     0.130897      12.88
 O      -2.474433     2.553217     0.309054     231.68
 C      -3.632546     2.806302     1.110791     103.08
 H      -4.182811     1.707805     1.014432      22.33
 H      -3.240617     2.829616     2.103319      26.77
 H      -3.980865     3.810055     0.867671      25.79
 C      -0.803034     0.872634     0.336518      12.71
 O       0.016404     1.801137     0.929792     113.30
 C      -0.186267    -0.251208    -0.296551      30.98
 H       0.729666    -0.313727     0.179206      19.55
 C      -2.505836    -0.971149    -0.809690     -13.29
 C      -3.444814    -2.114429    -1.466986      77.67
 H      -4.444871    -1.732701    -2.094560      22.86
 O      -2.592591    -2.784911    -2.432677     207.59
 H      -2.850654    -3.825849    -2.410384      16.61
 C      -3.879722    -3.042024    -0.312921     106.14
 H      -3.014366    -3.611528     0.061761      20.92
 O      -4.209429    -2.289610     0.895669     305.21
 H      -3.354441    -1.944416     1.267731      26.02
 C      -4.704739    -4.251331    -0.416638      78.66
 O      -3.988218    -5.090677    -1.534964     263.78
 H      -4.598672    -5.722927    -2.134231      29.49
 H      -5.703472    -3.869398    -0.946496      23.04
 H      -4.624933    -4.830036     0.569447      25.39
55
name = lig-etoh-frame_211
 C       2.787693     1.498181    -2.222488      60.91
 H       2.178664     1.901529    -3.041446      22.03
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 C       3.405847     0.764832     0.011979      48.75
 H       3.246876     0.899451     1.104370      18.47
 C       4.005561    -0.496017    -0.543007       7.45
 O       4.665730    -1.600272     0.257093     180.70
 C       4.818175    -1.264860     1.731227     104.47
 H       3.908943    -0.901941     2.034900      27.77
 H       5.575129    -0.459743     2.065830      26.43
 H       5.034036    -2.361738     2.142156      25.53
 C       4.095476    -0.644013    -1.988352      11.11
 O       4.734067    -1.735829    -2.564925     231.36
 H       4.994945    -2.480136    -2.118237      21.92
 C       3.488329     0.310682    -2.769559      74.79
 H       3.545565     0.176588    -3.910423      25.85
 C       2.846237     1.830053    -0.788027      69.84
 C       2.242536     3.003221    -0.196159     139.80
 H       2.404211     3.872344    -0.661801      25.86
 O       2.543342     3.097271     1.249975     290.59
 H       3.473741     3.569395     1.314096      28.95
 C       0.689439     2.964128    -0.050852      41.10
 H       0.255434     2.714226    -1.074728      22.48
 C       0.194472     4.280320     0.557726      77.56
 O       0.530525     5.439883    -0.504177     192.73
 H       0.330228     5.314088    -1.429431      29.61
 H       0.589349     4.842369     1.510409      23.59
 H      -1.003365     4.358781     0.565893      22.29
 C      -0.996328    -1.177797    -0.989247      40.72
 H      -0.408523    -2.047398    -1.338319      24.78
 C      -2.947375     0.436610    -0.357305      27.83
 H      -4.120098     0.625701    -0.396748      23.75
 C      -2.139764     1.315898     0.174756      24.82
 O      -2.486231     2.576582     0.318081     256.29
 C      -3.646303     2.774408     1.090859     120.70
 H      -4.146601     1.874991     1.153714      28.00
 H      -3.228864     2.733208     2.181309      25.43
 H      -4.392746     3.630710     0.957631      26.10
 C      -0.801816     0.858778     0.285805      17.13
 O       0.066394     1.791362     0.940723      90.59
 C      -0.270734    -0.262512    -0.243141      39.00
 H       0.936713    -0.312538     0.016751      17.95
 C      -2.464576    -1.039584    -0.896166     -23.48
 C      -3.523583    -2.094483    -1.504041      85.17
 H      -4.286394    -1.811468    -2.100413      25.34
 O      -2.591956    -2.812822    -2.463876     222.42
 H      -2.873233    -3.795079    -2.429813      19.18
 C      -3.836672    -3.082821    -0.229426      88.70
 H      -2.824172    -3.533952    -0.046110      21.54
 O      -4.276447    -2.329332     0.903227     327.73
 H      -3.514348    -2.031898     1.428494      27.12
 C      -4.791078    -4.179888    -0.386015      97.62
 O      -3.962790    -5.047759    -1.531831     289.26
 H      -4.638994    -5.592229    -1.810316      34.80
 H      -5.726496    -4.007813    -0.762093      26.38
 H      -4.662822    -4.910281     0.521135      24.97
55
name = lig-etoh-frame_212
 C       2.783584     1.552993    -2.173593      47.55
 H       1.977051     1.840194    -2.881725      21.11
 C       3.427660     0.790315     0.011138      32.78
 H       3.491368     0.917802     1.148423      19.05
 C       4.015662    -0.486119    -0.509795       0.90
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 O       4.622436    -1.575315     0.292330     216.68
 C       4.826309    -1.300885     1.614256     126.79
 H       3.783774    -0.998986     2.150722      25.26
 H       5.510364    -0.561874     1.974101      28.65
 H       5.039595    -2.270002     1.843445      28.16
 C       4.127052    -0.606381    -1.982116       3.21
 O       4.660922    -1.780309    -2.600668     184.28
 H       5.137652    -2.501802    -1.994743      20.88
 C       3.518377     0.293060    -2.786257      69.73
 H       3.585065    -0.048148    -3.783092      26.78
 C       2.800327     1.793435    -0.825004      49.22
 C       2.125227     2.899593    -0.144284     133.13
 H       2.492239     3.989956    -0.620852      20.04
 O       2.590447     3.139017     1.186136     324.43
 H       3.448317     3.507596     1.223034      32.02
 C       0.685407     2.960546    -0.000190      73.06
 H       0.130185     2.723933    -0.890540      23.74
 C       0.194106     4.296394     0.515379     108.33
 O       0.480344     5.474937    -0.477775     222.96
 H       0.345154     5.220876    -1.434034      28.44
 H       0.464565     4.609842     1.444301      27.34
 H      -0.796828     4.049468     0.680091      25.20
 C      -1.084846    -1.187236    -0.949204      46.25
 H      -0.550176    -1.978223    -1.336943      25.16
 C      -2.982150     0.371436    -0.447033      33.37
 H      -3.983729     0.505376    -0.251835      24.95
 C      -2.117476     1.277287     0.194553       4.14
 O      -2.498784     2.671369     0.319350     223.46
 C      -3.665676     2.738887     1.159170     117.85
 H      -4.520542     1.791932     1.208808      23.83
 H      -3.406541     2.927358     2.166625      27.19
 H      -4.478182     3.403179     0.842591      26.83
 C      -0.763307     0.942109     0.268162      16.09
 O       0.146756     1.805963     0.933773     153.87
 C      -0.290950    -0.278995    -0.175803      44.87
 H       0.760257    -0.426565    -0.495037      21.94
 C      -2.441040    -1.011788    -0.991266      -1.84
 C      -3.492593    -2.095708    -1.506144      65.49
 H      -4.462417    -1.610046    -2.094423      21.90
 O      -2.618427    -2.848719    -2.482850     240.72
 H      -2.930317    -3.726420    -2.478223      24.32
 C      -3.753170    -3.070021    -0.147191      76.19
 H      -2.710473    -3.429615    -0.144676      22.84
 O      -4.350843    -2.360448     0.913530     271.91
 H      -3.608256    -2.142694     1.718022      23.09
 C      -4.814176    -4.193244    -0.407691      81.10
 O      -3.967858    -4.983154    -1.501958     282.53
 H      -4.727641    -5.630199    -1.678141      31.39
 H      -6.043059    -4.085194    -0.581284      23.98
 H      -4.901878    -4.850596     0.448634      26.25
55
name = lig-etoh-frame_213
 C       2.796424     1.508071    -2.215424      37.96
 H       1.966988     2.091050    -2.663378      18.87
 C       3.492855     0.749533     0.008797      56.15
 H       3.635933     0.981937     1.012373      21.05
 C       4.029600    -0.428504    -0.484644      25.19
 O       4.562582    -1.495876     0.242296     243.33
 C       4.781184    -1.339458     1.569992     123.08
 H       3.948141    -1.223299     2.181525      27.65
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 H       5.661933    -0.576130     1.716893      26.39
 H       5.255782    -2.367860     2.032852      25.61
 C       4.177314    -0.640386    -1.901970      12.13
 O       4.585302    -1.807953    -2.631097     177.78
 H       5.150716    -2.267350    -1.905720      22.45
 C       3.502293     0.358280    -2.775887      62.99
 H       3.443120    -0.005393    -3.860572      23.59
 C       2.787551     1.679090    -0.843923      45.93
 C       2.077996     2.892501    -0.089451     128.34
 H       2.293633     3.645272    -0.740690      27.03
 O       2.637204     3.162537     1.157178     301.31
 H       3.627745     3.568333     1.074698      27.22
 C       0.621271     2.927551     0.042373      83.15
 H       0.074032     2.804350    -0.927239      23.45
 C       0.164369     4.342006     0.436096     101.91
 O       0.423763     5.490010    -0.424279     249.48
 H       0.397794     4.965194    -1.362234      27.19
 H       0.731685     4.432678     1.525432      23.44
 H      -0.947049     4.002599     0.647235      21.98
 C      -1.165515    -1.174853    -0.867348      18.49
 H      -0.784073    -2.260700    -1.348023      21.09
 C      -2.989244     0.214171    -0.542040      51.52
 H      -4.120896     0.365994    -0.330068      23.28
 C      -2.095212     1.253599     0.161637      -8.61
 O      -2.529096     2.733188     0.334092     172.60
 C      -3.757743     2.688196     1.241953     112.70
 H      -4.270240     1.827617     1.218341      28.33
 H      -3.553621     3.161272     2.287272      25.05
 H      -4.312995     3.488747     0.638836      25.13
 C      -0.691692     1.047298     0.288016       7.92
 O       0.237665     1.841477     0.917030     202.14
 C      -0.297586    -0.310598    -0.178177      37.34
 H       0.756321    -0.455384    -0.588628      21.65
 C      -2.517949    -0.908127    -1.068057      38.96
 C      -3.412681    -2.081732    -1.503152      89.15
 H      -4.301114    -1.630425    -1.755460      26.12
 O      -2.674384    -2.868122    -2.482216     208.88
 H      -3.128524    -3.864655    -2.562064      18.97
 C      -3.723357    -3.029366    -0.125295      81.97
 H      -2.730092    -3.482100     0.108679      23.70
 O      -4.395873    -2.374123     0.962282     318.28
 H      -3.838363    -2.263687     1.659611      32.09
 C      -4.789110    -4.236906    -0.455095      86.31
 O      -4.038310    -4.918769    -1.453378     262.98
 H      -4.512026    -5.810875    -1.799269      29.55
 H      -5.737472    -3.879830    -0.681281      27.30
 H      -4.976993    -4.869251     0.558900      25.66
55
name = lig-etoh-frame_214
 C       2.790634     1.431372    -2.272945      42.37
 H       2.250541     2.280977    -2.736618      17.86
 C       3.546061     0.726143    -0.003078      60.05
 H       3.689269     1.087946     1.109415      19.05
 C       4.076791    -0.396381    -0.510587      40.89
 O       4.498785    -1.434295     0.153852     238.32
 C       4.813933    -1.398901     1.602745     123.76
 H       3.881852    -1.209839     2.303181      25.35
 H       5.522729    -0.620337     1.602577      28.60
 H       5.338563    -2.181655     1.974507      29.08
 C       4.162430    -0.630168    -1.890185      31.69
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 O       4.517607    -1.801818    -2.612279     231.19
 H       5.099599    -2.261780    -2.070484      26.08
 C       3.489075     0.398268    -2.745828      66.28
 H       3.292842     0.283094    -3.794401      23.72
 C       2.789852     1.556050    -0.794648      53.08
 C       2.103704     2.872943    -0.101863     108.67
 H       2.178699     3.663997    -1.064652      22.54
 O       2.706552     3.185413     1.158161     308.00
 H       3.558416     3.616909     0.975409      30.01
 C       0.543958     2.912427     0.021585      90.03
 H       0.215020     2.742253    -1.021543      21.38
 C       0.109547     4.362110     0.458567     116.82
 O       0.368556     5.460497    -0.384936     308.82
 H       0.491883     5.153900    -1.249112      33.68
 H       0.725677     4.500442     1.226997      27.97
 H      -0.952927     4.470359     0.581632      24.77
 C      -1.200091    -1.194308    -0.796601      44.78
 H      -0.989207    -2.084950    -1.130693      22.80
 C      -3.024071     0.196757    -0.549368      42.28
 H      -4.104639     0.279249    -0.636229      19.50
 C      -2.078988     1.267071     0.087990     -15.31
 O      -2.570020     2.709020     0.372569     151.08
 C      -3.836067     2.732878     1.288151      85.60
 H      -4.099554     1.490686     1.303052      21.84
 H      -3.659052     3.080229     2.268629      26.69
 H      -4.318582     3.468287     0.659898      24.55
 C      -0.663702     1.058637     0.300327       0.68
 O       0.306463     1.881791     0.908027     212.96
 C      -0.294514    -0.311871    -0.227343      31.29
 H       0.895626    -0.491567    -0.243843      19.73
 C      -2.580687    -0.887734    -1.143719      44.25
 C      -3.318135    -2.085635    -1.444295      78.78
 H      -4.456737    -1.710408    -1.725101      25.41
 O      -2.757755    -2.892190    -2.477523     251.66
 H      -3.260146    -3.692890    -2.500865      23.56
 C      -3.729281    -3.012450    -0.127062      83.33
 H      -2.904673    -3.496646     0.446521      24.59
 O      -4.439877    -2.377143     0.996077     283.08
 H      -3.751162    -2.262858     1.776959      26.22
 C      -4.712424    -4.251314    -0.456710      87.04
 O      -4.118989    -4.901453    -1.441925     329.04
 H      -4.243902    -5.717940    -1.760745      35.44
 H      -5.576457    -3.546660    -1.013219      25.00
 H      -4.851181    -4.797095     0.412232      28.17
55
name = lig-etoh-frame_215
 C       2.751659     1.415472    -2.214171     117.35
 H       2.616670     2.209966    -2.994995      26.18
 C       3.570839     0.766457     0.040909      55.06
 H       3.654610     0.976453     1.029437      19.55
 C       4.148621    -0.388403    -0.597810      24.82
 O       4.471136    -1.465865     0.129547     202.95
 C       4.834391    -1.406231     1.621390      97.54
 H       3.964709    -1.177709     2.216473      25.51
 H       5.440183    -0.409897     1.774160      25.57
 H       5.457396    -2.416076     1.799520      24.05
 C       4.090358    -0.573071    -1.974804      22.54
 O       4.447944    -1.766885    -2.571379     213.47
 H       5.139757    -2.503109    -2.216891      22.17
 C       3.499935     0.370632    -2.746387      54.26
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 H       3.410227     0.343908    -3.854109      18.47
 C       2.762590     1.513535    -0.764410      67.97
 C       2.152875     2.862833    -0.201803     122.45
 H       2.330840     3.627543    -0.855801      23.49
 O       2.760199     3.207644     1.146810     296.12
 H       3.609061     3.736262     1.026173      29.25
 C       0.540631     2.949724    -0.058289      67.16
 H       0.228772     2.591709    -1.053482      22.21
 C       0.032603     4.360935     0.497163      85.76
 O       0.337091     5.451034    -0.375664     256.27
 H       0.581911     5.352393    -1.386356      27.59
 H       0.731101     4.678275     1.469917      22.43
 H      -1.029644     4.640048     0.792804      22.90
 C      -1.222195    -1.181841    -0.749503      19.64
 H      -0.798734    -2.354522    -0.993404      18.60
 C      -3.070143     0.328121    -0.515182      19.37
 H      -4.148573     0.524016    -0.774780      19.38
 C      -2.088858     1.321566     0.015861      -4.93
 O      -2.605664     2.622277     0.425103     183.91
 C      -3.872687     2.724900     1.279996     102.77
 H      -4.190400     1.813006     1.421598      28.75
 H      -3.631905     3.005297     2.380456      25.66
 H      -4.722729     3.349898     0.810919      25.18
 C      -0.697734     0.973645     0.285713      -8.16
 O       0.310678     1.883083     0.910212     153.42
 C      -0.259420    -0.265702    -0.249856      44.59
 H       0.735521    -0.580432     0.080759      19.70
 C      -2.524107    -0.929334    -1.167702      29.13
 C      -3.355307    -2.123878    -1.371887     100.13
 H      -4.291070    -1.926175    -1.753868      27.41
 O      -2.830940    -2.897712    -2.474401     240.23
 H      -3.421311    -3.743277    -2.403568      19.40
 C      -3.729550    -3.032412    -0.078998      94.38
 H      -2.866978    -3.442008     0.442095      26.08
 O      -4.474623    -2.365114     1.022626     273.65
 H      -3.660366    -2.167129     1.694896      24.85
 C      -4.669184    -4.134492    -0.464385     100.00
 O      -4.138168    -4.916591    -1.509428     282.27
 H      -4.240467    -5.939669    -1.571274      29.29
 H      -5.490188    -3.682832    -0.850842      28.45
 H      -4.958349    -4.822112     0.509145      25.04
55
name = lig-etoh-frame_216
 C       2.739613     1.410119    -2.131069      85.39
 H       2.651310     2.124964    -2.913867      26.01
 C       3.595216     0.768520     0.051463      61.76
 H       3.622977     0.869784     1.223043      17.15
 C       4.195845    -0.346287    -0.643275      13.93
 O       4.490788    -1.544736     0.154703     207.91
 C       4.878078    -1.375678     1.587809     116.55
 H       3.900594    -1.359885     2.212140      25.14
 H       5.423044    -0.550622     1.922918      28.73
 H       5.324064    -2.321308     1.651100      26.46
 C       4.050094    -0.575165    -2.043606      16.99
 O       4.384748    -1.748328    -2.555335     203.00
 H       5.003848    -2.452614    -2.219108      21.58
 C       3.475046     0.368862    -2.814627      56.83
 H       3.718592     0.219103    -3.894160      19.19
 C       2.705513     1.583026    -0.767615      77.60
 C       2.205801     2.871991    -0.261637     121.05
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 H       2.674322     3.822023    -0.889804      20.70
 O       2.785574     3.215541     1.110867     257.41
 H       3.649490     3.833328     1.124900      27.97
 C       0.592157     2.991429    -0.119676      53.46
 H       0.061394     2.657398    -1.048925      22.85
 C      -0.005071     4.374123     0.547394      98.16
 O       0.324122     5.482466    -0.392918     253.49
 H       0.548218     5.190629    -1.369085      27.57
 H       0.473264     4.514741     1.431935      27.13
 H      -1.053528     4.268272     0.964253      24.78
 C      -1.170716    -1.221691    -0.741435      32.42
 H      -0.771745    -2.103357    -0.758965      21.13
 C      -3.056610     0.451282    -0.531439      33.92
 H      -4.064529     0.944992    -0.748531      20.24
 C      -2.162045     1.369872    -0.032928       5.55
 O      -2.644455     2.531340     0.485546     201.73
 C      -3.881301     2.717295     1.267277     101.06
 H      -4.538048     1.623123     1.527966      23.53
 H      -3.532189     3.079043     2.222830      26.57
 H      -4.841034     3.178073     1.006307      25.86
 C      -0.742315     0.912377     0.262434      -6.33
 O       0.249183     1.847181     0.897824     115.31
 C      -0.245865    -0.217950    -0.244651      47.56
 H       0.649581    -0.764086     0.386181      18.08
 C      -2.472584    -0.906564    -1.078684      15.67
 C      -3.443129    -2.179404    -1.311360      69.48
 H      -4.507575    -1.799322    -1.733405      24.05
 O      -2.892386    -2.914727    -2.470602     215.82
 H      -3.344746    -3.873918    -2.430639      18.74
 C      -3.704229    -3.043128    -0.000255      97.05
 H      -2.664305    -3.422380     0.250235      25.14
 O      -4.474520    -2.340436     1.040172     307.78
 H      -3.818516    -2.019362     1.566581      31.71
 C      -4.660570    -4.057868    -0.434906      92.71
 O      -4.134381    -4.967688    -1.623156     253.24
 H      -4.284212    -5.859849    -1.058938      26.25
 H      -5.830841    -3.700200    -0.673582      25.06
 H      -4.956143    -4.616639     0.340318      27.79
55
name = lig-etoh-frame_217
 C       2.769796     1.389365    -2.137058      49.68
 H       2.261396     2.319064    -2.652794      20.18
 C       3.593698     0.750816     0.031766      56.29
 H       3.592356     0.765209     1.085212      20.11
 C       4.202872    -0.317850    -0.612635      15.40
 O       4.544913    -1.583845     0.168739     225.12
 C       4.867886    -1.361089     1.531734     118.73
 H       3.984833    -1.585637     2.165741      25.36
 H       5.632128    -0.552617     1.917982      25.81
 H       5.429362    -2.370724     1.795360      25.25
 C       4.044580    -0.605125    -2.022361      16.46
 O       4.328680    -1.772001    -2.590093     189.50
 H       4.880821    -2.271666    -2.007465      23.97
 C       3.431090     0.396941    -2.891115      56.81
 H       3.724646     0.278883    -3.913706      22.77
 C       2.707170     1.648630    -0.745270      54.95
 C       2.259670     2.985281    -0.271579     116.85
 H       2.704974     3.663105    -0.938538      24.97
 O       2.782546     3.209261     1.069346     319.63
 H       3.565204     3.730740     1.065127      31.21
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 C       0.641716     3.023231    -0.129561      45.38
 H       0.033442     2.925391    -1.030485      23.53
 C      -0.010508     4.343803     0.543557      95.38
 O       0.305013     5.513763    -0.400874     243.59
 H       0.399008     4.984692    -1.162492      32.62
 H       0.597146     4.448269     1.579720      24.25
 H      -1.056770     3.960450     0.694874      23.86
 C      -1.106232    -1.203301    -0.740032      24.69
 H      -0.715920    -2.386818    -0.716056      20.98
 C      -3.013332     0.505632    -0.622809      56.75
 H      -3.957076     0.978858    -0.747046      23.74
 C      -2.203978     1.379077    -0.036947      17.97
 O      -2.691996     2.486676     0.550898     225.21
 C      -3.916703     2.618390     1.290067     116.81
 H      -4.313608     1.771201     1.548789      29.87
 H      -3.491478     3.183602     2.159896      25.73
 H      -4.667600     3.345766     0.778170      25.83
 C      -0.789853     0.976607     0.248645       1.25
 O       0.152322     1.806481     0.859753     128.25
 C      -0.243646    -0.264060    -0.197606      42.82
 H       0.576329    -0.570399     0.250065      20.77
 C      -2.501058    -0.868602    -0.931974     -11.29
 C      -3.541224    -2.162482    -1.290549      74.19
 H      -4.460721    -1.663313    -1.423014      25.90
 O      -2.946727    -2.936510    -2.453815     249.12
 H      -3.137738    -3.830366    -2.472734      22.67
 C      -3.667335    -3.013998     0.034776     104.42
 H      -2.704610    -3.435436     0.246446      25.43
 O      -4.450738    -2.322709     1.041251     267.64
 H      -3.797604    -1.704405     1.684402      24.97
 C      -4.718148    -4.041248    -0.451788      80.00
 O      -4.164354    -5.024990    -1.672012     261.36
 H      -4.063788    -5.640577    -1.020954      28.32
 H      -5.605502    -3.594503    -0.642335      28.12
 H      -4.852374    -4.843732     0.511079      25.11
55
name = lig-etoh-frame_218
 C       2.768258     1.445829    -2.195310      60.10
 H       2.012194     2.116169    -2.483616      15.33
 C       3.546154     0.755411    -0.009622      61.80
 H       3.601746     0.778271     1.115067      19.28
 C       4.185878    -0.363062    -0.577780      33.46
 O       4.618923    -1.564775     0.148093     255.99
 C       4.897189    -1.418724     1.513643     132.35
 H       4.020045    -1.414309     2.195441      26.27
 H       5.517197    -0.561376     1.646529      28.20
 H       5.549135    -2.181766     1.908558      27.79
 C       4.018102    -0.577010    -1.988112      18.17
 O       4.295090    -1.825839    -2.636725     161.04
 H       4.771038    -2.252155    -1.766736      22.54
 C       3.410112     0.406007    -2.891296      34.70
 H       3.427197     0.463136    -4.053739      22.25
 C       2.797654     1.639574    -0.732232      51.93
 C       2.272292     3.080710    -0.230652     101.55
 H       2.603662     3.850240    -1.139565      25.14
 O       2.748207     3.196533     1.032342     297.94
 H       3.695036     3.703965     1.015946      26.94
 C       0.678664     3.067380    -0.099125      35.26
 H       0.212065     3.028306    -1.132128      21.63
 C       0.044441     4.279387     0.538139     103.07
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 O       0.272600     5.518006    -0.374701     173.25
 H       0.272644     4.946128    -1.297058      27.42
 H       0.487700     4.527703     1.479965      26.07
 H      -1.037467     4.035869     0.344980      22.64
 C      -1.088989    -1.220737    -0.732031      46.99
 H      -0.926769    -2.223960    -0.869269      24.06
 C      -2.976887     0.454963    -0.762261      49.18
 H      -4.142948     0.667445    -0.886096      24.53
 C      -2.154673     1.376202     0.016381      14.50
 O      -2.717453     2.486354     0.607424     214.97
 C      -3.938925     2.579827     1.311248      99.71
 H      -4.329578     1.428553     1.706917      23.02
 H      -3.705683     3.213395     2.231495      25.04
 H      -4.328472     3.275142     0.561554      23.61
 C      -0.831705     1.060973     0.207880      20.25
 O       0.065946     1.809147     0.806480     107.26
 C      -0.290501    -0.291392    -0.130041      12.92
 H       0.984955    -0.355980     0.085560      17.43
 C      -2.557795    -0.861580    -0.806965      -6.29
 C      -3.547034    -2.087367    -1.255393      56.47
 H      -4.621758    -1.598157    -1.366617      23.53
 O      -2.998807    -2.900534    -2.426205     173.10
 H      -3.121469    -3.999145    -2.273133      13.97
 C      -3.674378    -2.978936     0.002080     102.48
 H      -2.756867    -3.461132     0.469974      22.96
 O      -4.399729    -2.293586     1.054897     293.51
 H      -3.814947    -1.666578     1.566077      27.71
 C      -4.730200    -4.118747    -0.435433      70.24
 O      -4.227906    -5.050917    -1.668141     206.37
 H      -3.609543    -5.788164    -1.120917      24.79
 H      -5.663158    -3.425172    -0.830334      24.14
 H      -4.798964    -4.793928     0.269696      28.12
55
name = lig-etoh-frame_219
 C       2.745542     1.517671    -2.206238      86.11
 H       1.868796     1.989605    -2.835134      21.68
 C       3.515600     0.735015     0.008657      53.26
 H       3.612210     0.962946     1.105848      21.58
 C       4.142799    -0.447633    -0.575424      29.29
 O       4.688273    -1.532052     0.092490     233.76
 C       4.946776    -1.461156     1.527471     115.05
 H       4.042919    -1.100661     2.156002      25.05
 H       5.405426    -0.372562     1.507135      25.34
 H       5.655179    -2.252651     1.871600      26.54
 C       3.984580    -0.556606    -2.014263      20.40
 O       4.283695    -1.856985    -2.628491     193.27
 H       4.591278    -2.511197    -1.980498      25.46
 C       3.386653     0.430598    -2.849839      37.01
 H       3.121045     0.376196    -3.857546      20.90
 C       2.892954     1.660286    -0.805812      46.07
 C       2.251693     3.093648    -0.231938     109.88
 H       2.329555     3.940187    -0.890022      25.75
 O       2.742086     3.223027     1.037492     330.96
 H       3.643384     3.576329     1.129771      29.18
 C       0.719100     3.087877    -0.086145      58.39
 H       0.453348     2.904510    -1.117051      22.23
 C       0.079177     4.253477     0.481944     106.48
 O       0.245537     5.478011    -0.352010     257.63
 H       0.206766     5.432910    -1.325835      30.61
 H       0.323262     4.589719     1.562603      24.33
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 H      -0.998919     4.236928     0.458329      23.67
 C      -1.160881    -1.220368    -0.696241      31.04
 H      -0.909230    -2.339850    -1.067624      22.25
 C      -2.977788     0.397582    -0.854479      41.21
 H      -3.989423     0.378051    -1.017179      25.58
 C      -2.163622     1.356935     0.060156       2.62
 O      -2.680991     2.498656     0.651166     200.36
 C      -3.963252     2.531598     1.343963     117.84
 H      -4.404038     1.649950     1.564899      29.04
 H      -3.964960     3.081316     2.284739      26.83
 H      -4.660377     3.007082     0.579489      25.72
 C      -0.836538     1.058801     0.136733      16.84
 O       0.038610     1.890532     0.766366     133.37
 C      -0.293814    -0.266555    -0.067171      42.05
 H       0.658107    -0.222698    -0.207903      23.52
 C      -2.579183    -0.918211    -0.763934      11.02
 C      -3.500864    -1.985291    -1.205294      87.78
 H      -4.501331    -1.737903    -1.520333      25.13
 O      -3.050856    -2.847568    -2.383597     230.05
 H      -3.318785    -3.652079    -1.998547      23.42
 C      -3.717044    -2.980938    -0.038194      98.45
 H      -2.849207    -3.354015     0.470434      24.65
 O      -4.359253    -2.263932     1.061796     322.15
 H      -3.663169    -1.767425     1.461896      30.73
 C      -4.705140    -4.175185    -0.471888      84.01
 O      -4.285274    -5.080485    -1.605721     288.89
 H      -3.411063    -5.552969    -1.568910      27.91
 H      -5.585262    -3.743540    -0.914159      25.53
 H      -5.043134    -4.954424     0.443039      23.89
55
name = lig-etoh-frame_220
 C       2.708502     1.566651    -2.228073      82.91
 H       2.140972     1.987291    -2.990305      27.42
 C       3.526976     0.689153     0.037908      64.22
 H       3.595209     1.080438     1.032960      23.28
 C       4.062135    -0.488569    -0.592909       9.34
 O       4.752367    -1.525203     0.030719     191.51
 C       5.000975    -1.394578     1.523127     114.60
 H       4.088256    -1.265281     2.055084      27.51
 H       5.555885    -0.488869     1.656689      28.13
 H       5.584369    -2.328506     1.776965      26.94
 C       3.967233    -0.605010    -2.050826      17.55
 O       4.268354    -1.853485    -2.619310     226.17
 H       4.479555    -2.648783    -2.136964      24.74
 C       3.346573     0.449950    -2.776104      70.48
 H       2.957480     0.019091    -3.798853      20.93
 C       2.933258     1.767154    -0.906629      47.29
 C       2.225973     3.019976    -0.217532     113.73
 H       2.342376     4.094399    -0.827030      20.75
 O       2.743040     3.263576     1.099276     313.10
 H       3.686221     3.622855     1.144114      28.35
 C       0.743063     3.028585    -0.100200      72.56
 H       0.421141     2.787699    -1.158169      22.07
 C       0.059896     4.310069     0.411444      99.99
 O       0.243471     5.469340    -0.325189     298.39
 H       0.153548     5.569544    -1.260017      30.51
 H       0.345471     4.525493     1.517270      23.61
 H      -1.064526     4.107374     0.687124      22.65
 C      -1.235749    -1.241743    -0.619034      54.39
 H      -0.746194    -2.094192    -1.098996      23.80
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 C      -2.967211     0.380418    -0.837344      39.25
 H      -4.126300     0.486117    -1.152568      23.81
 C      -2.269401     1.311427     0.044777     -17.95
 O      -2.627927     2.516424     0.697014     148.18
 C      -4.010237     2.511316     1.322560      99.32
 H      -4.492773     1.349491     1.505346      23.86
 H      -4.043040     3.051236     2.352253      25.12
 H      -4.978932     2.759354     0.844265      25.83
 C      -0.797684     1.027924     0.094571      -2.37
 O       0.058304     2.013582     0.736841     146.90
 C      -0.362193    -0.244386    -0.081459      44.43
 H       0.872354    -0.282857    -0.392799      20.56
 C      -2.537262    -0.981049    -0.795294      35.54
 C      -3.465499    -1.949936    -1.180723      90.02
 H      -4.449757    -1.559432    -1.591509      24.12
 O      -3.085031    -2.762724    -2.331842     226.83
 H      -3.535885    -3.609703    -2.062641      23.87
 C      -3.788156    -3.005078    -0.054715      76.09
 H      -2.731920    -3.382775     0.229767      24.28
 O      -4.341945    -2.235740     1.058560     280.77
 H      -3.362491    -1.939943     1.533118      22.22
 C      -4.667480    -4.277199    -0.479237     102.37
 O      -4.331354    -5.100113    -1.548088     319.56
 H      -3.410428    -5.302556    -1.620122      30.76
 H      -5.724590    -3.927109    -0.974962      23.72
 H      -5.100025    -4.657508     0.362306      27.56
55
name = lig-etoh-frame_221
 C       2.708002     1.577432    -2.281372      68.03
 H       2.256544     2.361627    -2.994118      26.98
 C       3.531496     0.688142    -0.019596      64.74
 H       3.635772     1.043817     1.091856      22.18
 C       3.987091    -0.485006    -0.610058      19.32
 O       4.813455    -1.523715    -0.006539     171.97
 C       5.055430    -1.324008     1.472109     114.94
 H       4.046672    -1.537559     2.017548      25.30
 H       5.849213    -0.542396     1.858184      25.91
 H       5.477934    -2.282609     1.716987      28.11
 C       3.938925    -0.671414    -2.030743      14.42
 O       4.248751    -1.823639    -2.649374     203.44
 H       4.433827    -2.657465    -1.989665      21.36
 C       3.294358     0.368487    -2.748243      67.77
 H       3.018222    -0.069259    -3.647720      21.76
 C       2.944374     1.878214    -0.909687      45.96
 C       2.251013     2.971467    -0.191710     112.93
 H       2.486170     3.838187    -0.769646      21.53
 O       2.742999     3.294572     1.186481     297.94
 H       3.666052     3.771621     1.008538      25.78
 C       0.698939     2.948458    -0.157726      76.46
 H       0.304443     2.818405    -1.153899      22.88
 C       0.004482     4.348623     0.374158      96.57
 O       0.261091     5.519358    -0.294598     246.58
 H       0.052269     5.284243    -1.341059      26.10
 H       0.589996     4.496100     1.340730      23.89
 H      -0.948709     3.951608     0.542128      24.30
 C      -1.215016    -1.262482    -0.520528      76.66
 H      -0.671070    -2.121643    -0.956331      22.88
 C      -3.013844     0.392740    -0.745359      64.84
 H      -3.905516     0.727111    -1.098328      27.43
 C      -2.324177     1.272311     0.004169     -18.59
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 O      -2.622785     2.518837     0.733113     113.87
 C      -4.093604     2.426727     1.324742     103.73
 H      -4.036720     1.408215     1.520704      26.77
 H      -3.915704     2.940870     2.213047      27.10
 H      -4.922227     2.909358     0.754887      26.11
 C      -0.792142     1.060192     0.117327     -17.56
 O       0.079024     2.099368     0.711773     198.17
 C      -0.362831    -0.241122    -0.175082      55.30
 H       0.612627    -0.495897    -0.194210      24.41
 C      -2.501380    -0.963597    -0.861326      23.78
 C      -3.536039    -2.000931    -1.206836      95.22
 H      -4.352614    -1.221363    -1.376546      24.66
 O      -3.091331    -2.694821    -2.293800     225.14
 H      -3.690968    -3.529212    -2.614295      22.84
 C      -3.830400    -3.027590    -0.070249      84.25
 H      -2.840741    -3.460930    -0.020860      26.43
 O      -4.293988    -2.220961     1.060664     319.28
 H      -3.609184    -2.206809     1.692244      30.49
 C      -4.711301    -4.289129    -0.481723      97.42
 O      -4.349877    -5.144610    -1.515518     257.19
 H      -3.276522    -5.212053    -1.431618      27.15
 H      -5.672782    -3.878738    -0.791770      25.63
 H      -4.984699    -4.760179     0.643119      25.22
55
name = lig-etoh-frame_222
 C       2.749392     1.586383    -2.310849      49.97
 H       2.379159     2.491233    -2.770901      17.47
 C       3.513223     0.771248    -0.107521      56.18
 H       3.691134     0.805839     0.910382      24.63
 C       3.967092    -0.486054    -0.619669      31.52
 O       4.863105    -1.488330    -0.012780     209.52
 C       5.103028    -1.310703     1.406929     127.87
 H       4.207694    -1.292947     1.947147      28.16
 H       5.792793    -0.593652     1.858312      28.26
 H       5.583445    -2.336010     1.657136      27.46
 C       3.865651    -0.690261    -1.970847      25.84
 O       4.239312    -1.823621    -2.690457     223.33
 H       4.436794    -2.361318    -1.936531      24.89
 C       3.224558     0.254638    -2.751359      41.51
 H       3.054266     0.023793    -3.886105      24.84
 C       2.962020     1.866731    -0.864131      53.65
 C       2.281076     2.961987    -0.138613     105.22
 H       2.572398     3.895958    -0.892937      20.89
 O       2.742227     3.313442     1.249742     328.23
 H       3.518700     3.823030     1.121939      29.65
 C       0.644585     2.950612    -0.251941      63.31
 H       0.273111     2.808027    -1.308321      20.38
 C       0.009975     4.330404     0.374520      85.49
 O       0.268345     5.592566    -0.323592     268.10
 H       0.124989     5.225402    -1.168007      31.00
 H       0.731758     4.400937     1.293855      22.65
 H      -1.129814     4.044855     0.380652      22.09
 C      -1.170338    -1.289741    -0.462841      33.98
 H      -0.788027    -2.404898    -0.615432      19.29
 C      -3.066972     0.377837    -0.637183      42.65
 H      -4.060080     0.850046    -1.078849      20.48
 C      -2.228789     1.326474     0.022698       1.52
 O      -2.666273     2.489094     0.733269     148.92
 C      -4.111493     2.354196     1.319718      85.24
 H      -4.026933     1.220813     1.598075      23.34
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 H      -3.861577     2.978042     2.296552      24.13
 H      -4.673217     2.946645     0.575214      24.09
 C      -0.828325     1.104675     0.168869       5.50
 O       0.063224     2.092373     0.707921     199.76
 C      -0.332748    -0.195961    -0.249330      28.91
 H       0.808536    -0.608794     0.043008      20.00
 C      -2.512556    -0.921700    -0.921596       7.77
 C      -3.652935    -2.017259    -1.214655      88.95
 H      -4.517671    -1.346169    -1.290768      26.48
 O      -3.082082    -2.672834    -2.339950     287.81
 H      -3.708751    -3.083492    -2.865668      30.55
 C      -3.848772    -3.035408    -0.106475      85.67
 H      -2.846917    -3.559243     0.075592      24.94
 O      -4.258550    -2.237146     1.053897     256.28
 H      -3.677561    -2.405808     1.941111      24.79
 C      -4.819550    -4.246106    -0.389199      94.34
 O      -4.319257    -5.195325    -1.495420     306.57
 H      -3.423038    -5.364461    -1.215541      31.09
 H      -5.851387    -3.775060    -0.649169      26.09
 H      -4.646031    -4.891268     0.415588      28.59
55
name = lig-etoh-frame_223
 C       2.838090     1.559252    -2.259687      56.10
 H       2.422942     2.382932    -2.850208      19.91
 C       3.521320     0.822234    -0.172096      59.13
 H       3.700900     0.804547     0.978415      22.32
 C       3.992998    -0.476613    -0.616816      27.39
 O       4.892062    -1.412157    -0.013107     226.33
 C       5.157991    -1.361038     1.354552     124.20
 H       4.194619    -0.978817     1.964712      24.29
 H       5.814789    -0.403332     1.601418      25.91
 H       5.644671    -2.243729     1.630426      28.42
 C       3.758746    -0.705175    -1.973425      17.18
 O       4.237244    -1.827094    -2.706697     194.72
 H       4.611578    -2.416974    -2.003565      24.62
 C       3.105045     0.235026    -2.810440      58.26
 H       3.192553     0.174251    -3.877499      27.55
 C       2.966173     1.765984    -0.841496      52.23
 C       2.297456     3.029966    -0.115260     103.23
 H       2.490323     3.886775    -0.734650      24.98
 O       2.711196     3.306431     1.280239     283.82
 H       3.587866     3.913868     1.322026      25.61
 C       0.617043     3.025688    -0.331116      50.51
 H       0.382151     2.717788    -1.351516      22.96
 C       0.045749     4.295549     0.366419      99.22
 O       0.272729     5.650807    -0.359795     238.60
 H       0.273440     5.462357    -1.364804      28.61
 H       0.458223     4.319490     1.380137      25.47
 H      -0.999043     4.351521     0.463950      25.25
 C      -1.179843    -1.303889    -0.464538      16.25
 H      -0.989611    -2.328700    -0.292188      20.51
 C      -3.090000     0.374100    -0.545552      22.22
 H      -4.076159     0.621112    -0.849925      20.92
 C      -2.125225     1.417512     0.074049      18.75
 O      -2.724146     2.443223     0.713863     214.11
 C      -4.027403     2.298634     1.332581     114.96
 H      -4.588678     1.301110     1.536051      25.52
 H      -4.119722     2.883263     2.184559      27.96
 H      -4.684636     2.698182     0.539603      25.89
 C      -0.832930     1.112002     0.200303      17.47
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 O       0.027551     2.026324     0.710227     178.02
 C      -0.256194    -0.163443    -0.265496      26.89
 H       0.716834    -0.281618     0.192006      22.74
 C      -2.568883    -0.898979    -0.923566       5.96
 C      -3.713831    -1.985280    -1.212708      72.03
 H      -4.849535    -1.723833    -1.459808      25.27
 O      -3.068409    -2.658322    -2.432302     220.28
 H      -3.860259    -2.792152    -3.073172      26.58
 C      -3.840684    -3.050934    -0.114662      94.83
 H      -2.928274    -3.515356     0.207797      25.50
 O      -4.243220    -2.267553     1.048868     236.05
 H      -3.643250    -2.558462     1.878342      25.28
 C      -4.889075    -4.199177    -0.316101      88.18
 O      -4.304417    -5.218676    -1.469357     240.38
 H      -3.505413    -5.595834    -1.011866      28.03
 H      -6.027626    -3.974901    -0.451014      26.76
 H      -4.683480    -4.980879     0.487115      27.01
55
name = lig-etoh-frame_224
 C       2.909278     1.507603    -2.207646      64.75
 H       2.466587     2.173971    -3.005913      22.30
 C       3.613697     0.734371    -0.088252      64.43
 H       3.609850     1.117910     0.906287      23.29
 C       4.029143    -0.446882    -0.640598      23.20
 O       4.897354    -1.335086    -0.044658     231.22
 C       5.200639    -1.326754     1.345401     126.13
 H       4.365617    -1.053754     1.922564      27.21
 H       5.897362    -0.487247     1.251247      26.52
 H       5.699501    -2.295702     1.736080      26.72
 C       3.655142    -0.748260    -2.036100       3.41
 O       4.230890    -1.827660    -2.693327     164.64
 H       4.869812    -2.551041    -2.241354      22.30
 C       3.006935     0.292157    -2.842459      72.12
 H       3.183518     0.180641    -3.937022      25.53
 C       2.902341     1.752736    -0.867474      55.56
 C       2.294507     3.092961    -0.113649      97.30
 H       2.572585     4.111183    -0.713971      24.13
 O       2.668793     3.290116     1.288890     297.55
 H       3.522382     3.781929     1.368240      28.17
 C       0.635297     3.098141    -0.319497      44.79
 H       0.431269     2.725475    -1.344233      23.81
 C       0.080261     4.310631     0.305162      92.65
 O       0.287885     5.684176    -0.392175     197.96
 H       0.529406     5.745571    -1.422630      27.14
 H       0.270452     4.353872     1.495469      23.28
 H      -1.065844     4.391571     0.508322      23.35
 C      -1.220181    -1.230175    -0.511275       7.68
 H      -1.041897    -2.324517    -0.024545      21.79
 C      -3.024300     0.386116    -0.459901      38.29
 H      -4.168762     0.490089    -0.549904      21.07
 C      -2.167261     1.419323     0.090155      23.96
 O      -2.770123     2.423606     0.719377     240.34
 C      -4.000282     2.246934     1.306090     131.18
 H      -4.631359     1.329717     1.478783      25.81
 H      -4.256620     2.923054     2.227683      26.13
 H      -4.815023     2.559744     0.607015      26.79
 C      -0.773407     1.076727     0.181623      11.71
 O       0.027401     1.977189     0.713082     135.54
 C      -0.258904    -0.168009    -0.234058      24.44
 H       0.854659    -0.140245     0.224853      21.82
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 C      -2.651706    -0.886855    -0.853609       3.37
 C      -3.717129    -1.976040    -1.249667      79.09
 H      -4.704619    -1.848499    -1.575871      27.16
 O      -3.081595    -2.642832    -2.536919     205.88
 H      -3.868080    -2.558620    -3.216243      26.78
 C      -3.853493    -3.061976    -0.090517      91.01
 H      -2.852399    -3.542392     0.111300      25.22
 O      -4.251222    -2.306175     1.052735     294.62
 H      -3.587557    -2.440827     1.661796      31.47
 C      -4.888393    -4.226694    -0.265390      94.36
 O      -4.310045    -5.208600    -1.426546     194.91
 H      -3.707651    -5.844295    -0.805430      26.25
 H      -5.971349    -4.096508    -0.395557      27.27
 H      -5.011675    -4.766952     0.726881      28.11
55
name = lig-etoh-frame_225
 C       2.898193     1.505864    -2.224936      44.46
 H       2.543782     2.230485    -2.900618      22.32
 C       3.658039     0.709302     0.020920      61.92
 H       3.752282     1.194312     1.022881      21.58
 C       4.056086    -0.430275    -0.699443       9.67
 O       4.895465    -1.310964    -0.106866     184.64
 C       5.271690    -1.257520     1.327680     112.08
 H       4.360167    -1.097500     2.062451      25.10
 H       6.155927    -0.533830     1.413135      26.55
 H       5.635112    -2.212513     1.629345      27.99
 C       3.589177    -0.780586    -2.086747      17.39
 O       4.220590    -1.841258    -2.699054     223.31
 H       4.870645    -2.349464    -2.278983      26.87
 C       2.998100     0.271841    -2.841298      76.75
 H       2.935663     0.187702    -3.974757      24.88
 C       2.859019     1.761329    -0.834641      48.34
 C       2.278665     3.146599    -0.152259     105.15
 H       2.716320     4.042667    -0.633335      25.42
 O       2.611339     3.255356     1.281390     318.92
 H       3.508276     3.667771     1.266790      28.68
 C       0.710688     3.122343    -0.247306      58.56
 H       0.378623     2.900772    -1.275232      23.89
 C       0.039955     4.407570     0.251877     112.52
 O       0.323087     5.713796    -0.411826     289.57
 H       0.673950     5.585352    -1.253699      33.46
 H       0.464782     4.500232     1.207313      26.68
 H      -0.995129     4.136001     0.204131      25.97
 C      -1.275800    -1.157501    -0.547953      41.52
 H      -1.009143    -2.070189    -0.231609      28.25
 C      -2.997020     0.406695    -0.401220      71.67
 H      -4.065633     0.551055    -0.153823      25.23
 C      -2.231702     1.321257     0.078387       9.96
 O      -2.784142     2.441794     0.746824     202.72
 C      -4.100055     2.230085     1.288332     107.80
 H      -4.059653     1.030925     1.586331      24.68
 H      -4.044046     2.852213     2.155717      27.06
 H      -4.802239     2.667879     0.578758      26.70
 C      -0.763434     1.056092     0.120593       2.43
 O       0.086333     1.981887     0.721302     139.25
 C      -0.307972    -0.201763    -0.166501      47.29
 H       0.824280    -0.392570    -0.057404      23.92
 C      -2.683002    -0.902157    -0.752279      -0.66
 C      -3.644765    -2.021557    -1.305677      64.55
 H      -4.697021    -1.493194    -1.630076      23.30
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 O      -3.114791    -2.613012    -2.631954     267.98
 H      -3.730030    -2.452378    -3.270872      30.32
 C      -3.870691    -3.080659    -0.080513      90.21
 H      -2.879549    -3.557329    -0.101174      25.17
 O      -4.281704    -2.344888     1.062886     253.56
 H      -3.331176    -2.100702     1.685687      22.47
 C      -4.846891    -4.301127    -0.235073      89.46
 O      -4.334055    -5.187527    -1.324947     263.10
 H      -3.965630    -5.896916    -0.871212      30.50
 H      -5.923041    -3.902138    -0.701243      24.26
 H      -5.058912    -4.604970     0.836093      26.57
55
name = lig-etoh-frame_226
 C       2.818081     1.546769    -2.232262      28.13
 H       2.533248     2.521399    -2.782767      18.36
 C       3.615102     0.784007     0.060396      60.91
 H       4.089979     0.863784     1.098280      24.28
 C       4.049645    -0.394641    -0.744955       6.38
 O       4.918439    -1.335750    -0.154245     150.46
 C       5.337329    -1.172601     1.293579     116.98
 H       4.532212    -0.965965     1.996020      26.97
 H       6.196932    -0.593804     1.732702      28.18
 H       5.630951    -2.271137     1.399757      26.54
 C       3.587988    -0.783683    -2.083109      21.26
 O       4.189278    -1.860030    -2.735923     214.39
 H       4.862506    -2.158798    -2.028227      24.33
 C       3.032113     0.209099    -2.843570      62.49
 H       2.696478     0.147537    -3.842720      25.02
 C       2.879181     1.745318    -0.756452      36.50
 C       2.266459     3.126426    -0.180748     111.90
 H       2.775840     4.042415    -0.750112      22.77
 O       2.558631     3.217533     1.257723     317.42
 H       3.553625     3.590995     1.255206      26.92
 C       0.784135     3.131877    -0.181379      70.86
 H       0.383628     2.996362    -1.192058      21.66
 C      -0.002381     4.511114     0.194761      94.51
 O       0.361963     5.731225    -0.426817     259.15
 H       0.789756     5.334016    -1.303923      28.19
 H       0.567237     4.743168     1.239351      21.77
 H      -1.033139     4.085013     0.004002      23.26
 C      -1.341642    -1.114859    -0.578547      44.38
 H      -0.901174    -2.272806    -0.735449      23.64
 C      -3.105633     0.353077    -0.377192      57.53
 H      -4.088881     0.613696    -0.085704      25.85
 C      -2.188173     1.300679     0.117415      -2.81
 O      -2.759066     2.461920     0.759367     167.76
 C      -4.161313     2.196718     1.297225     104.38
 H      -3.970910     1.228358     1.619710      27.96
 H      -4.007876     2.803929     2.243894      25.58
 H      -4.849758     2.594827     0.539124      25.91
 C      -0.787510     1.099827     0.074811       5.67
 O       0.173530     2.020622     0.711062     143.65
 C      -0.370559    -0.242985    -0.118587      46.02
 H       0.680041    -0.667015    -0.235667      24.27
 C      -2.652889    -0.950916    -0.675910      24.05
 C      -3.600374    -2.041850    -1.365816      81.45
 H      -4.361982    -1.349744    -1.480041      25.26
 O      -3.134837    -2.578492    -2.688364     248.26
 H      -3.811764    -2.301250    -3.408517      26.77
 C      -3.875977    -3.107405    -0.119760      82.37
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 H      -2.862486    -3.580277    -0.043834      24.83
 O      -4.276369    -2.373934     1.099742     288.34
 H      -3.592935    -1.913585     1.491779      30.65
 C      -4.824668    -4.319307    -0.263209     114.19
 O      -4.373086    -5.166686    -1.197232     267.54
 H      -4.019777    -6.059489    -0.891715      27.66
 H      -5.648582    -3.830644    -0.760798      25.42
 H      -5.003134    -4.707505     0.796399      26.60
55
name = lig-etoh-frame_227
 C       2.719018     1.566560    -2.185368      49.39
 H       2.443319     2.445907    -2.690006      24.07
 C       3.578571     0.822931     0.022003      70.16
 H       4.108513     0.693239     0.904927      25.77
 C       4.022560    -0.340108    -0.743991      10.04
 O       4.955423    -1.345520    -0.181818     163.70
 C       5.404943    -1.149667     1.250944     117.81
 H       4.494275    -0.844933     1.879481      25.33
 H       6.232660    -0.485681     1.583382      27.95
 H       5.638593    -2.204114     1.368652      27.08
 C       3.641426    -0.761585    -2.045739      21.39
 O       4.160979    -1.890823    -2.753254     203.44
 H       4.781048    -2.131873    -1.933475      22.73
 C       3.035320     0.253530    -2.830142      51.17
 H       2.540499    -0.030321    -3.871148      20.05
 C       2.920190     1.747568    -0.711488      31.30
 C       2.298406     3.057889    -0.175030     122.71
 H       2.630121     3.905823    -0.857409      24.37
 O       2.543146     3.193630     1.226694     362.01
 H       3.403352     3.508872     1.399191      31.29
 C       0.779542     3.154300    -0.161108      69.33
 H       0.481821     2.903126    -1.211182      21.05
 C       0.008501     4.568834     0.211857     100.68
 O       0.417906     5.735720    -0.490926     291.36
 H       0.754395     5.472685    -1.425161      28.72
 H       0.018675     4.757409     1.250374      25.98
 H      -1.081653     4.421961     0.083471      24.73
 C      -1.314180    -1.200207    -0.609321      48.26
 H      -1.039816    -1.948973    -1.259426      24.72
 C      -3.214017     0.279485    -0.340482      22.62
 H      -4.375500     0.542950    -0.321858      23.35
 C      -2.162881     1.335694     0.178169     -15.01
 O      -2.718229     2.469293     0.754788     143.70
 C      -4.131783     2.224087     1.326188      81.49
 H      -4.396658     0.995286     1.729392      24.06
 H      -4.317334     2.847729     2.247217      25.61
 H      -4.950675     2.340115     0.598237      26.33
 C      -0.760347     1.159542     0.078165       9.14
 O       0.254621     2.066082     0.674816     167.42
 C      -0.432641    -0.251335    -0.100020      33.66
 H       0.658610    -0.747746    -0.313679      22.34
 C      -2.681791    -0.996794    -0.659149      18.12
 C      -3.556076    -2.044785    -1.374932      69.54
 H      -4.521562    -1.316685    -1.502846      23.61
 O      -3.152327    -2.539082    -2.725568     229.70
 H      -3.878462    -2.137933    -3.351891      25.84
 C      -3.828568    -3.122427    -0.159596      84.18
 H      -2.860413    -3.545703     0.180889      24.22
 O      -4.296625    -2.414675     1.102355     223.82
 H      -3.520681    -1.809142     1.459973      24.95
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 C      -4.816922    -4.263862    -0.262991     100.94
 O      -4.391360    -5.205691    -1.122860     236.77
 H      -3.965727    -6.106950    -0.775758      25.79
 H      -5.890926    -3.751621    -0.675072      23.96
 H      -5.028234    -4.795047     0.658656      26.26
55
name = lig-etoh-frame_228
 C       2.642179     1.520401    -2.101802      61.54
 H       2.179502     2.328335    -2.765487      25.87
 C       3.591982     0.767865    -0.062067      65.65
 H       3.934385     0.957323     1.074560      22.32
 C       4.022418    -0.335017    -0.719935      23.27
 O       4.987579    -1.314385    -0.195689     204.67
 C       5.442919    -1.159775     1.197243     117.97
 H       4.510632    -0.824526     1.742657      24.97
 H       6.253951    -0.343423     1.084627      26.50
 H       5.766286    -2.141965     1.629917      26.97
 C       3.699147    -0.693314    -2.047364      15.41
 O       4.135538    -1.906184    -2.714330     217.05
 H       4.722323    -2.433683    -2.214230      27.44
 C       2.987407     0.354196    -2.798502      58.70
 H       2.710262     0.006375    -3.713294      21.38
 C       2.918229     1.800281    -0.752587      47.15
 C       2.330284     2.990962    -0.139997     117.49
 H       2.634310     3.887985    -0.855425      22.19
 O       2.545033     3.178217     1.216530     332.27
 H       3.456645     3.554279     1.486818      27.04
 C       0.715733     3.176414    -0.195861      63.20
 H       0.506571     2.899801    -1.219924      21.97
 C       0.020753     4.585773     0.239352      92.24
 O       0.493513     5.749337    -0.571742     283.49
 H       0.620205     5.612886    -1.500216      30.56
 H      -0.333757     4.768566     1.375617      22.89
 H      -1.096897     4.606543    -0.019364      22.92
 C      -1.283157    -1.285577    -0.639956      40.44
 H      -0.916442    -1.862595    -1.620389      22.33
 C      -3.256360     0.236735    -0.278480      37.86
 H      -4.234317     0.363148    -0.576192      22.93
 C      -2.220711     1.339469     0.217813     -20.99
 O      -2.710494     2.471687     0.769634     152.42
 C      -4.105437     2.218934     1.377057     107.23
 H      -4.435197     1.267350     1.697105      28.06
 H      -4.435398     2.961336     2.107066      27.25
 H      -4.824983     2.265292     0.567888      27.24
 C      -0.709218     1.181159     0.130471      -4.24
 O       0.298829     2.087808     0.631805     179.53
 C      -0.445744    -0.241386    -0.132189      22.07
 H       0.629005    -0.422416    -0.192790      23.97
 C      -2.740866    -1.004703    -0.694366       3.87
 C      -3.579162    -2.022850    -1.338985      83.01
 H      -4.571117    -1.770140    -1.557299      26.62
 O      -3.169341    -2.490462    -2.743271     258.25
 H      -3.814189    -2.084558    -3.225749      31.06
 C      -3.759689    -3.114831    -0.152066      93.95
 H      -2.815848    -3.537234     0.191275      24.66
 O      -4.324056    -2.447349     1.072712     211.82
 H      -3.434700    -1.951171     1.488194      23.23
 C      -4.863055    -4.173964    -0.247468      99.92
 O      -4.390369    -5.301692    -1.122913     257.30
 H      -3.919313    -5.830342    -0.519643      30.26
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 H      -5.882058    -3.863875    -0.489627      27.27
 H      -5.095681    -4.651751     0.799464      26.56
55
name = lig-etoh-frame_229
 C       2.550986     1.502993    -2.071051      61.81
 H       1.887557     2.095272    -2.683959      24.56
 C       3.616478     0.760567    -0.082252      76.26
 H       3.617662     1.152837     0.854818      24.53
 C       4.085115    -0.417987    -0.699810      30.43
 O       5.006130    -1.288990    -0.207345     230.12
 C       5.464909    -1.149310     1.113492     130.60
 H       4.665350    -0.768303     1.783447      27.32
 H       6.145420    -0.368996     0.942972      28.86
 H       5.948238    -1.944264     1.743864      27.76
 C       3.754206    -0.610463    -2.084944      25.54
 O       4.090108    -1.884395    -2.667640     171.43
 H       4.696464    -2.672892    -2.368811      20.49
 C       2.972324     0.386106    -2.718023      74.79
 H       2.799527     0.245094    -3.892944      24.30
 C       2.901347     1.805296    -0.812150      59.03
 C       2.322135     3.012512    -0.120961     120.41
 H       2.765923     3.926875    -0.645825      20.65
 O       2.574054     3.168131     1.253266     313.46
 H       3.492363     3.641473     1.332670      26.26
 C       0.668651     3.195051    -0.247505      57.80
 H       0.341741     3.057190    -1.325214      21.55
 C      -0.016194     4.593877     0.221514      93.74
 O       0.585081     5.771963    -0.608906     196.88
 H       0.417759     5.463920    -1.658528      25.05
 H       0.042738     4.829957     1.238706      25.76
 H      -0.957584     4.439296    -0.321388      22.92
 C      -1.289841    -1.315129    -0.694936      53.27
 H      -0.746869    -1.892742    -1.389410      23.89
 C      -3.193473     0.221309    -0.207053      52.56
 H      -4.272865     0.433387    -0.675034      18.47
 C      -2.278635     1.294071     0.230285     -15.80
 O      -2.743344     2.473147     0.818933     152.36
 C      -4.092263     2.257773     1.381816      79.74
 H      -4.131104     1.088961     1.991729      22.44
 H      -4.302974     3.224902     1.997309      25.00
 H      -4.640422     2.385653     0.407596      24.34
 C      -0.744188     1.141554     0.205335      -7.70
 O       0.287991     2.066753     0.599247     156.60
 C      -0.422644    -0.200272    -0.198901       7.86
 H       0.808585    -0.121590    -0.044404      21.23
 C      -2.725096    -0.978284    -0.753518       8.74
 C      -3.642934    -2.045765    -1.294735      66.52
 H      -4.810917    -2.006686    -1.481919      23.88
 O      -3.165843    -2.447443    -2.726597     201.83
 H      -3.865178    -1.979336    -3.303185      26.46
 C      -3.728458    -3.109108    -0.116272      85.72
 H      -2.720497    -3.618824     0.020289      24.27
 O      -4.319995    -2.454920     1.032345     254.49
 H      -3.651616    -2.216385     1.612711      29.61
 C      -4.876572    -4.151167    -0.230836      73.22
 O      -4.404065    -5.384282    -1.121138     193.10
 H      -3.724702    -5.611743    -0.364167      27.27
 H      -6.017845    -3.795761    -0.604560      24.79
 H      -4.987435    -4.364504     0.817673      27.34
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name = lig-etoh-frame_230
 C       2.429364     1.514980    -2.106131      48.63
 H       1.626556     2.073935    -2.599591      21.84
 C       3.624808     0.805803    -0.110255      51.86
 H       3.587973     1.112323     1.058410      21.14
 C       4.141290    -0.459894    -0.699143      33.57
 O       5.021309    -1.324983    -0.224347     227.24
 C       5.487745    -1.090609     1.065155     124.08
 H       4.772051    -0.688208     1.888723      25.45
 H       6.270804    -0.187141     1.128534      25.99
 H       6.059656    -1.940623     1.430625      28.31
 C       3.828829    -0.580494    -2.093142      39.48
 O       4.022909    -1.839779    -2.655234     192.74
 H       4.703615    -2.463423    -2.211307      21.44
 C       2.991023     0.335427    -2.710372      79.84
 H       2.847583     0.488359    -3.713998      29.58
 C       2.880020     1.762652    -0.810913      45.08
 C       2.277298     3.094875    -0.125651     110.76
 H       2.822267     4.021113    -0.557244      23.73
 O       2.628715     3.161656     1.314382     319.40
 H       3.406453     3.664933     1.247451      30.22
 C       0.666042     3.213203    -0.300119      65.96
 H       0.254030     3.144802    -1.291294      23.59
 C      -0.014292     4.593534     0.114664      89.71
 O       0.662577     5.764444    -0.637195     227.38
 H       0.491012     5.459326    -1.503256      31.46
 H       0.370673     4.886328     1.171162      24.06
 H      -1.051466     4.362415    -0.235382      24.77
 C      -1.287125    -1.240521    -0.728012      23.89
 H      -0.704252    -2.206931    -1.102094      21.03
 C      -3.118804     0.243128    -0.173296      60.58
 H      -4.077620     0.585602    -0.307566      20.16
 C      -2.287385     1.255408     0.250565       7.76
 O      -2.768492     2.455515     0.875708     211.44
 C      -4.069751     2.317353     1.373969     121.43
 H      -4.012345     1.473160     1.994778      27.41
 H      -4.161684     3.194791     1.942098      27.49
 H      -4.764142     2.305636     0.520347      25.65
 C      -0.868004     1.063101     0.264394       6.90
 O       0.225749     2.017489     0.573469     127.53
 C      -0.359766    -0.137044    -0.260878      21.72
 H       0.653872    -0.285885    -0.172549      23.92
 C      -2.654224    -0.962626    -0.819078      17.45
 C      -3.732211    -2.091546    -1.270283      79.85
 H      -4.732119    -1.747967    -1.300678      28.36
 O      -3.167933    -2.409050    -2.681574     194.91
 H      -3.817097    -1.955943    -3.364283      26.22
 C      -3.731318    -3.131121    -0.110274      96.70
 H      -2.786623    -3.627145    -0.039347      27.18
 O      -4.300394    -2.436381     0.992344     199.33
 H      -3.695667    -2.419507     1.958495      22.23
 C      -4.878316    -4.179909    -0.273494      85.16
 O      -4.427537    -5.428728    -1.061562     223.30
 H      -3.454091    -5.630157    -0.695389      27.38
 H      -5.725714    -3.745706    -0.716729      27.69
 H      -4.988160    -4.397081     0.880580      26.80
55
name = lig-etoh-frame_231
 C       2.344327     1.487756    -2.140062      31.53
 H       1.531996     2.117642    -2.596422      19.48
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 C       3.652293     0.834579    -0.092009      56.48
 H       3.829391     0.831715     0.910264      24.06
 C       4.141751    -0.375343    -0.730383      31.40
 O       5.040869    -1.392647    -0.226615     218.76
 C       5.563436    -0.992865     1.083908     125.05
 H       4.759325    -0.847341     1.791291      27.70
 H       6.213876    -0.199931     1.147824      29.23
 H       6.085048    -2.013778     1.103799      26.26
 C       3.888628    -0.590203    -2.067899      34.84
 O       3.969582    -1.798595    -2.664088     216.15
 H       4.651490    -2.097134    -2.096350      23.97
 C       2.989338     0.334441    -2.730078      70.93
 H       2.852092     0.290650    -3.890318      27.30
 C       2.806013     1.755848    -0.789696      50.47
 C       2.228372     3.155807    -0.127137     112.15
 H       2.753169     4.076268    -0.633861      23.29
 O       2.670069     3.153472     1.360367     265.25
 H       3.524713     3.786944     1.363283      26.23
 C       0.680384     3.220463    -0.325618      54.57
 H       0.367589     2.968131    -1.393234      20.88
 C       0.047430     4.595420     0.012800     105.48
 O       0.716645     5.724768    -0.645578     224.60
 H       0.743273     5.581504    -1.705593      27.38
 H       0.273125     4.785362     1.063097      25.82
 H      -1.096019     4.619220     0.176627      24.88
 C      -1.216457    -1.134284    -0.763439      33.22
 H      -1.046198    -2.216224    -0.651806      23.86
 C      -3.053478     0.254726    -0.185142      42.26
 H      -4.173894     0.561610     0.074868      19.63
 C      -2.261903     1.265017     0.310871      28.57
 O      -2.746692     2.420999     0.899628     226.90
 C      -4.059813     2.406006     1.349046     110.19
 H      -4.219755     1.493405     2.315486      22.96
 H      -4.230281     3.361864     2.042134      24.32
 H      -4.994934     2.161541     0.782853      24.57
 C      -0.933254     1.008690     0.279210      19.63
 O       0.131153     1.973619     0.555807     104.13
 C      -0.365081    -0.121276    -0.324307      22.44
 H       0.801462    -0.570333    -0.391024      21.12
 C      -2.618759    -0.955835    -0.851646       0.84
 C      -3.740338    -2.077807    -1.255479      77.35
 H      -4.674525    -1.356832    -1.243871      24.80
 O      -3.193213    -2.386666    -2.621660     260.59
 H      -3.726389    -2.020872    -3.251852      30.76
 C      -3.775678    -3.176102    -0.143125      93.74
 H      -2.736815    -3.622556     0.079402      25.14
 O      -4.262534    -2.390563     0.999084     258.10
 H      -3.722256    -2.575482     1.755970      28.69
 C      -4.810503    -4.277897    -0.301195      95.05
 O      -4.441028    -5.444259    -0.988174     303.48
 H      -3.557288    -5.664562    -1.024972      32.77
 H      -5.687269    -3.659037    -0.991419      23.27
 H      -5.220491    -4.612138     0.614923      28.53
55
name = lig-etoh-frame_232
 C       2.323707     1.423087    -2.135443      63.19
 H       1.678187     2.050723    -2.698909      23.61
 C       3.683024     0.839442    -0.097050      65.91
 H       4.092123     0.845518     1.007313      21.98
 C       4.157364    -0.265748    -0.761922      19.34
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 O       5.032953    -1.409418    -0.222507     184.27
 C       5.645373    -0.977038     1.095571     110.52
 H       4.710452    -1.124601     1.785069      24.78
 H       6.274461     0.028607     1.017573      25.80
 H       6.228454    -1.851372     1.313023      28.17
 C       3.837263    -0.536167    -2.082555      26.24
 O       3.952944    -1.775259    -2.676005     151.64
 H       4.760984    -2.231503    -2.119370      21.00
 C       2.969528     0.375085    -2.793606      37.30
 H       2.830841    -0.153577    -3.740892      22.26
 C       2.698507     1.782552    -0.767409      68.89
 C       2.213942     3.153340    -0.102122     110.58
 H       2.596518     4.027826    -0.686048      21.65
 O       2.702348     3.163640     1.369238     296.21
 H       3.483394     3.749958     1.509745      28.25
 C       0.665991     3.191563    -0.352233      50.10
 H       0.618124     2.802043    -1.343147      22.15
 C       0.106506     4.601466    -0.032739     110.83
 O       0.758819     5.673285    -0.673111     270.02
 H       1.013708     5.678011    -1.667566      28.11
 H       0.337384     4.692806     1.106300      23.84
 H      -0.922862     4.842478     0.137442      25.36
 C      -1.200031    -1.087037    -0.796174      70.25
 H      -1.039930    -2.147800    -0.558080      24.57
 C      -3.071970     0.254933    -0.218347      54.16
 H      -4.052730     0.133143     0.181139      24.41
 C      -2.251098     1.271748     0.374739      12.62
 O      -2.712511     2.397833     0.907662     212.65
 C      -4.100510     2.477984     1.437728     129.16
 H      -4.294658     1.738357     2.265322      27.30
 H      -4.274922     3.399872     1.819201      28.53
 H      -4.910563     2.160952     0.790120      27.33
 C      -0.849245     1.021168     0.238254      21.74
 O       0.037578     1.961962     0.559476     138.47
 C      -0.348081    -0.167465    -0.383621      51.95
 H       0.608879    -0.312023    -0.422219      24.35
 C      -2.622775    -0.915418    -0.820725     -14.85
 C      -3.667640    -1.978726    -1.238290      83.71
 H      -4.560314    -1.412304    -1.302194      24.30
 O      -3.227614    -2.395222    -2.550578     259.59
 H      -3.853399    -2.007080    -3.251293      27.89
 C      -3.814349    -3.206715    -0.157862      94.45
 H      -2.834233    -3.523994     0.102104      25.15
 O      -4.235139    -2.349256     0.991515     280.62
 H      -3.539734    -2.548101     1.739446      26.14
 C      -4.771309    -4.350928    -0.360603     114.65
 O      -4.459332    -5.483105    -0.946707     272.69
 H      -3.444318    -5.613648    -1.216013      27.78
 H      -5.535586    -3.921707    -0.962952      24.54
 H      -5.521149    -4.664209     0.501421      25.66
55
name = lig-etoh-frame_233
 C       2.336278     1.382352    -2.101491      83.77
 H       1.771160     2.039537    -2.854060      23.69
 C       3.686567     0.885129    -0.087592      45.41
 H       4.082334     1.212620     0.850156      23.32
 C       4.215971    -0.218401    -0.790889       2.93
 O       5.011832    -1.363011    -0.212120     185.76
 C       5.697430    -1.005886     1.088106     120.22
 H       4.972693    -1.034935     1.848374      27.31
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 H       5.998494    -0.008343     1.004564      28.48
 H       6.563510    -1.637231     1.576111      26.19
 C       3.727234    -0.463921    -2.124762      21.50
 O       3.980362    -1.763045    -2.671475     208.29
 H       4.629452    -2.427179    -2.432836      25.71
 C       2.968004     0.361155    -2.846228      37.03
 H       2.589028    -0.201510    -3.718441      21.58
 C       2.639529     1.778421    -0.740657      62.69
 C       2.224378     3.086112    -0.044590     118.63
 H       2.549898     4.033561    -0.716269      19.99
 O       2.700717     3.174517     1.344939     326.38
 H       3.486747     3.758610     1.411547      28.08
 C       0.645816     3.127736    -0.349014      43.01
 H       0.615742     2.765777    -1.410852      19.08
 C       0.159294     4.594035    -0.013982     100.22
 O       0.830826     5.654664    -0.702063     263.51
 H       0.968717     5.410366    -1.605189      31.26
 H       0.581659     4.647822     1.003448      24.01
 H      -0.968423     4.778869    -0.283405      23.12
 C      -1.266046    -1.152976    -0.841635      75.50
 H      -0.706386    -2.179085    -0.903227      23.82
 C      -3.125229     0.264080    -0.217032      56.84
 H      -4.157381    -0.076208     0.134392      19.96
 C      -2.235915     1.212219     0.389767     -12.01
 O      -2.699496     2.411614     0.940110     150.60
 C      -4.130918     2.523461     1.507956      88.47
 H      -4.252427     1.792100     2.569358      22.93
 H      -4.285620     3.697497     1.608959      24.45
 H      -4.677209     2.253637     0.557772      24.71
 C      -0.768928     1.058906     0.138392       9.59
 O      -0.004968     2.021149     0.593155     170.98
 C      -0.329425    -0.150137    -0.404002      24.80
 H       0.928978    -0.089366    -0.384577      17.67
 C      -2.613158    -0.866964    -0.760353      26.68
 C      -3.563484    -1.891457    -1.208010      72.33
 H      -4.684990    -1.539090    -1.328400      23.97
 O      -3.263793    -2.423394    -2.508621     237.85
 H      -3.983484    -2.040987    -3.159430      26.14
 C      -3.826827    -3.164033    -0.142540      70.65
 H      -2.766102    -3.591939     0.029597      23.03
 O      -4.220404    -2.336888     0.980354     284.23
 H      -3.415097    -2.197860     1.745788      21.40
 C      -4.827584    -4.351160    -0.385860      91.89
 O      -4.422016    -5.605957    -0.959091     261.87
 H      -3.454238    -5.448356    -1.220803      29.46
 H      -5.693381    -3.954898    -1.196459      22.99
 H      -5.335697    -4.448989     0.527167      28.30
55
name = lig-etoh-frame_234
 C       2.347110     1.406401    -2.087478      84.42
 H       1.767585     2.041801    -2.691343      25.22
 C       3.664491     0.965866    -0.108460      45.88
 H       4.017300     1.514562     0.815547      21.04
 C       4.272073    -0.199085    -0.799953      11.98
 O       4.996308    -1.287172    -0.197201     208.32
 C       5.722175    -1.036647     1.081839     117.45
 H       5.058222    -0.918815     2.065328      24.67
 H       5.875819     0.123280     1.023358      25.12
 H       6.705864    -1.420763     1.305407      27.46
 C       3.710822    -0.510522    -2.112752      20.30
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 O       3.990511    -1.739732    -2.691673     225.58
 H       4.684933    -2.369073    -2.449628      26.37
 C       2.926039     0.339213    -2.885297      37.14
 H       2.358456     0.189746    -3.855904      20.69
 C       2.669985     1.715400    -0.730798      31.59
 C       2.221990     3.003452    -0.020960     122.56
 H       2.626499     3.857068    -0.553387      20.00
 O       2.672497     3.183645     1.304344     311.36
 H       3.541621     3.788937     1.174446      24.83
 C       0.651210     3.056510    -0.311723      72.66
 H       0.371279     2.855534    -1.355569      19.60
 C       0.188088     4.562248     0.004789      97.34
 O       0.927992     5.644139    -0.735597     244.78
 H       0.809264     5.146786    -1.712397      24.34
 H       0.457877     4.744018     1.064914      23.85
 H      -0.811134     4.486544    -0.320710      24.16
 C      -1.237481    -1.226885    -0.872387      58.68
 H      -0.799696    -2.034656    -1.404407      23.07
 C      -3.186464     0.297173    -0.153382      57.75
 H      -4.294381     0.227354     0.029977      22.17
 C      -2.237509     1.162282     0.369659     -14.20
 O      -2.681868     2.431421     0.998101     140.40
 C      -4.121969     2.566614     1.535491     112.86
 H      -4.275734     2.047496     2.508243      26.27
 H      -4.270961     3.609411     1.522242      26.89
 H      -4.632549     2.218640     0.621900      25.93
 C      -0.797883     1.087113     0.030132      -1.81
 O       0.006082     2.149222     0.637587     199.33
 C      -0.274400    -0.115457    -0.418752      36.08
 H       0.722496    -0.213126    -0.466240      22.13
 C      -2.585087    -0.874548    -0.725439      19.35
 C      -3.550804    -1.883604    -1.181394      87.25
 H      -4.569843    -1.546331    -1.192175      25.59
 O      -3.290623    -2.460528    -2.502768     298.94
 H      -3.970698    -2.150642    -3.011851      31.41
 C      -3.769586    -3.080797    -0.128618      77.40
 H      -2.887367    -3.684172    -0.038613      23.81
 O      -4.212760    -2.332161     0.989473     326.58
 H      -3.564533    -2.055523     1.639746      27.92
 C      -4.933573    -4.293102    -0.454359      68.62
 O      -4.359337    -5.718580    -0.975750     241.01
 H      -3.496592    -5.495278    -1.150807      32.65
 H      -5.657161    -3.966777    -1.098998      26.51
 H      -5.156635    -4.365199     0.716487      26.30
55
name = lig-etoh-frame_235
 C       2.368814     1.438219    -2.100444      33.88
 H       1.592704     2.189983    -2.491254      19.98
 C       3.690904     1.005595    -0.135320      55.47
 H       4.019944     1.484093     0.830300      20.44
 C       4.277992    -0.164186    -0.788789      34.25
 O       4.992176    -1.214898    -0.172767     241.09
 C       5.703179    -0.960358     1.082056     119.64
 H       5.168676    -1.205027     1.966177      26.81
 H       5.954945     0.081429     1.069792      26.89
 H       6.682062    -1.550854     0.871900      25.72
 C       3.757324    -0.609244    -2.079138      23.45
 O       3.995377    -1.732420    -2.735054     162.49
 H       4.868225    -2.086775    -2.207696      22.45
 C       2.832477     0.369410    -2.866759      47.93
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 H       2.533083     0.453542    -3.886256      24.60
 C       2.729100     1.653760    -0.753877      42.53
 C       2.189299     2.905074    -0.067370     126.13
 H       2.769299     3.808048    -0.653865      21.13
 O       2.646548     3.195489     1.271688     324.58
 H       3.436861     3.687235     1.193989      29.87
 C       0.691529     3.042019    -0.233860      93.84
 H       0.250625     2.867900    -1.226592      19.51
 C       0.242205     4.516487     0.030411      87.28
 O       1.008607     5.584888    -0.776783     257.33
 H       0.865532     5.456603    -1.738381      28.56
 H       0.045570     4.875579     1.127517      24.19
 H      -0.914459     4.424979    -0.160095      23.19
 C      -1.148431    -1.194343    -0.867954      43.16
 H      -1.114240    -1.935327    -1.798999      20.71
 C      -3.207311     0.295679    -0.084088      45.65
 H      -4.253116     0.626001    -0.036732      19.69
 C      -2.264011     1.211054     0.351990      -2.66
 O      -2.649677     2.429673     1.066760     157.46
 C      -4.059289     2.592160     1.475070     109.00
 H      -4.413498     2.191041     2.686219      23.15
 H      -4.257443     3.704929     1.579882      25.13
 H      -4.878430     2.082266     0.902737      25.24
 C      -0.861370     1.135789    -0.013695     -11.15
 O       0.002846     2.257491     0.666274     171.41
 C      -0.281838    -0.125442    -0.461559      22.56
 H       0.889837    -0.401954    -0.611163      20.18
 C      -2.568711    -0.910619    -0.712763     -13.81
 C      -3.592810    -1.953444    -1.161186      79.61
 H      -4.592924    -1.333716    -1.121501      22.85
 O      -3.296588    -2.502023    -2.504872     250.42
 H      -4.086675    -2.225513    -3.066026      26.69
 C      -3.715094    -3.010412    -0.148569      73.73
 H      -2.845960    -3.722830     0.054269      21.10
 O      -4.241346    -2.341938     0.998823     236.88
 H      -3.454130    -2.044029     1.800669      19.91
 C      -4.949696    -4.244767    -0.472786      47.69
 O      -4.333399    -5.768124    -0.980794     122.67
 H      -3.272110    -5.591536    -1.043820      25.46
 H      -5.973611    -3.904887    -1.141597      23.94
 H      -5.191764    -4.495560     0.510392      28.12
55
name = lig-etoh-frame_236
 C       2.360437     1.484229    -2.123814      52.01
 H       1.608022     2.171576    -2.405300      19.71
 C       3.796927     0.969459    -0.137360      56.18
 H       4.096056     1.217174     0.852829      21.75
 C       4.240730    -0.157704    -0.793337      20.58
 O       4.985015    -1.143140    -0.147555     226.20
 C       5.713698    -0.884794     1.045223     121.99
 H       5.211801    -1.573485     1.884544      24.83
 H       6.103145     0.167094     1.233836      25.99
 H       6.421928    -1.657754     0.724667      25.35
 C       3.739438    -0.582500    -2.072733      15.22
 O       4.053457    -1.761482    -2.759770     215.95
 H       4.799070    -2.018027    -2.265115      26.74
 C       2.779868     0.388638    -2.778105      56.62
 H       2.868304     0.354304    -3.943803      27.10
 C       2.749058     1.652103    -0.793933      47.89
 C       2.203600     2.856239    -0.161877     125.97
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 H       2.559756     3.607587    -0.817562      24.54
 O       2.602116     3.184347     1.251722     291.01
 H       3.494815     3.699459     1.281749      27.01
 C       0.738770     3.099386    -0.166736      85.42
 H       0.406611     2.829147    -1.196944      21.11
 C       0.247696     4.511054     0.046687     106.48
 O       1.067935     5.513713    -0.764388     262.84
 H       0.930727     5.525498    -1.799013      26.01
 H       0.141163     4.886293     1.032060      26.66
 H      -0.774965     4.571584    -0.249698      25.79
 C      -1.142282    -1.108391    -0.882701      74.21
 H      -1.084309    -1.776899    -1.643325      24.56
 C      -3.159361     0.243005    -0.042801      54.60
 H      -4.202717     0.748733    -0.156484      16.68
 C      -2.278152     1.329271     0.346924       5.43
 O      -2.628332     2.403839     1.127434     189.35
 C      -4.013113     2.618748     1.441316     130.51
 H      -4.205669     2.272707     2.585017      25.26
 H      -4.204558     3.710223     1.490242      26.51
 H      -4.888855     2.064051     1.121151      26.19
 C      -0.881203     1.183053     0.015519     -25.46
 O      -0.053122     2.286201     0.700720     157.80
 C      -0.281308    -0.130455    -0.517027      39.04
 H       0.791886    -0.240328    -0.698160      22.21
 C      -2.582666    -0.922769    -0.691897      -9.09
 C      -3.643009    -1.992051    -1.176357      88.09
 H      -4.525612    -1.346941    -1.216810      24.33
 O      -3.304790    -2.535301    -2.509600     257.10
 H      -4.137402    -2.391301    -3.134233      25.80
 C      -3.721371    -3.031933    -0.146288      85.62
 H      -2.789174    -3.507087     0.117099      23.34
 O      -4.258801    -2.347154     1.039429     291.53
 H      -3.642916    -2.351823     1.682327      31.23
 C      -4.911670    -4.220252    -0.508446      72.86
 O      -4.323245    -5.743267    -0.989760     189.13
 H      -3.340671    -5.761233    -0.767065      26.65
 H      -5.743313    -3.978376    -0.985376      27.29
 H      -5.375893    -4.636761     0.488764      26.16
55
name = lig-etoh-frame_237
 C       2.335066     1.533984    -2.118203      63.74
 H       1.617025     2.211660    -2.654712      19.41
 C       3.872523     0.939516    -0.159406      68.17
 H       4.164205     0.963563     0.982388      21.52
 C       4.195158    -0.214723    -0.815961      21.54
 O       4.964899    -1.068120    -0.152855     234.84
 C       5.735680    -0.881492     1.016334     130.53
 H       5.254275    -1.406249     1.779572      28.71
 H       6.115621     0.062451     1.463123      27.19
 H       6.652822    -1.551070     0.888193      27.01
 C       3.666257    -0.482782    -2.101097      19.17
 O       4.121722    -1.771155    -2.763948     185.90
 H       4.914376    -2.298395    -2.373701      21.96
 C       2.824171     0.331176    -2.728086      59.64
 H       2.919683     0.107254    -3.733943      28.00
 C       2.788611     1.668369    -0.794213      68.53
 C       2.241767     2.876876    -0.192410     112.04
 H       2.425540     3.766035    -1.041805      20.20
 O       2.569290     3.164532     1.221087     272.47
 H       3.477710     3.646972     1.294754      27.38
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 C       0.745059     3.138489    -0.150644      63.76
 H       0.550164     2.876331    -1.184024      21.52
 C       0.256588     4.562768     0.019652     100.85
 O       1.122048     5.453757    -0.714963     207.34
 H       0.900522     5.177664    -1.719620      26.19
 H       0.560970     4.884545     1.133211      22.88
 H      -0.760078     4.668639    -0.481900      24.00
 C      -1.239622    -1.020909    -0.905890      54.43
 H      -0.689543    -1.972532    -1.483148      22.61
 C      -3.078916     0.224858    -0.036291      63.37
 H      -4.121253     0.325016    -0.179315      18.85
 C      -2.251535     1.397136     0.330576      11.59
 O      -2.615876     2.377297     1.167171     189.89
 C      -3.992780     2.652795     1.463040     110.91
 H      -3.796979     2.405930     2.649189      22.32
 H      -4.165119     3.715637     1.271646      26.58
 H      -4.713098     2.006824     0.907668      25.31
 C      -0.851344     1.220680     0.095124     -14.81
 O      -0.135636     2.253879     0.732535     156.49
 C      -0.294661    -0.024901    -0.540411      40.87
 H       0.803900    -0.003395    -0.768903      21.36
 C      -2.621839    -0.907908    -0.669153      19.41
 C      -3.651311    -1.974940    -1.224346      73.72
 H      -4.690799    -1.497685    -1.344441      24.97
 O      -3.315343    -2.564407    -2.520744     317.75
 H      -4.051650    -2.589336    -3.051141      29.54
 C      -3.809716    -3.119320    -0.105637      78.59
 H      -2.714491    -3.389458     0.078624      23.28
 O      -4.295495    -2.362394     1.055862     241.88
 H      -3.592650    -2.626200     1.920145      21.22
 C      -4.783543    -4.273869    -0.477738      76.08
 O      -4.331184    -5.660308    -0.998752     249.37
 H      -3.538985    -5.817597    -0.452677      29.90
 H      -5.675219    -3.879895    -1.326777      24.03
 H      -5.377088    -4.510407     0.419972      26.74
55
name = lig-etoh-frame_238
 C       2.334305     1.524968    -2.120670      55.83
 H       1.800436     2.167931    -2.841101      20.94
 C       3.871741     0.937582    -0.180411      83.33
 H       4.094192     0.984694     0.801057      24.24
 C       4.148577    -0.250800    -0.823849      30.91
 O       4.979500    -1.048581    -0.179264     244.16
 C       5.783777    -0.918616     1.014368     119.92
 H       5.100954    -1.264256     1.941511      25.87
 H       5.959717     0.116125     1.413064      26.59
 H       6.801657    -1.317363     1.026459      27.71
 C       3.692893    -0.515971    -2.096044      21.91
 O       4.174214    -1.740689    -2.760730     178.19
 H       4.906213    -2.397996    -2.419112      21.35
 C       2.852224     0.316649    -2.737755      50.57
 H       2.607311    -0.070580    -3.827944      23.37
 C       2.844583     1.716905    -0.779100      82.21
 C       2.259651     2.989629    -0.167108     130.87
 H       2.549567     3.801889    -0.756699      24.67
 O       2.567270     3.150263     1.185198     318.16
 H       3.404045     3.541741     1.251586      31.66
 C       0.706549     3.114664    -0.181771      43.01
 H       0.365751     2.878768    -1.241252      23.36
 C       0.302517     4.634435     0.024894     122.02
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 O       1.174019     5.401748    -0.692421     292.08
 H       1.065324     5.098219    -1.572513      32.20
 H       0.501612     4.801033     1.003577      28.22
 H      -0.759016     4.730715    -0.243964      27.03
 C      -1.275629    -0.973860    -0.960387      52.90
 H      -0.688860    -1.814107    -0.977706      27.13
 C      -3.022591     0.269014    -0.046473      62.57
 H      -4.172613    -0.039307     0.087048      18.76
 C      -2.220770     1.360302     0.301776      17.25
 O      -2.589691     2.374335     1.185831     197.05
 C      -3.960295     2.677595     1.509790     111.42
 H      -3.981249     2.549007     2.645741      24.70
 H      -4.190025     3.730816     1.058061      25.87
 H      -4.482799     1.988007     0.825996      25.04
 C      -0.813641     1.235455     0.175446      22.88
 O      -0.182025     2.226478     0.751237     173.33
 C      -0.358167     0.148775    -0.532212      18.35
 H       0.792699     0.110294    -0.848864      21.54
 C      -2.651032    -0.917499    -0.692519       9.67
 C      -3.672797    -1.954807    -1.250211      74.89
 H      -4.745177    -1.660629    -1.392199      25.74
 O      -3.295214    -2.588149    -2.526215     268.80
 H      -4.150182    -2.781842    -3.018210      25.34
 C      -3.870819    -3.178507    -0.070130      82.19
 H      -2.833443    -3.485168     0.018934      25.44
 O      -4.325349    -2.408179     1.078704     295.85
 H      -3.806656    -2.550309     1.903918      26.18
 C      -4.700628    -4.345295    -0.481814     104.05
 O      -4.324820    -5.534837    -0.998098     241.57
 H      -3.821094    -5.976212    -0.128151      27.32
 H      -5.159324    -3.953932    -1.244387      29.84
 H      -5.363646    -4.377956     0.476375      27.10
55
name = lig-etoh-frame_239
 C       2.397996     1.448622    -2.134193      71.78
 H       1.897180     2.191269    -2.747198      25.21
 C       3.787606     0.964360    -0.224409      59.70
 H       4.100120     1.230717     0.900064      20.78
 C       4.129201    -0.239717    -0.791158      32.49
 O       5.056154    -1.115408    -0.204711     246.73
 C       5.777850    -0.911140     1.070307     122.82
 H       5.179414    -1.269113     1.873505      28.41
 H       5.763350     0.224515     1.076731      25.13
 H       6.730355    -1.454822     1.001992      27.41
 C       3.792839    -0.662001    -2.091038      23.98
 O       4.206100    -1.695761    -2.770031     223.45
 H       4.821443    -2.165651    -2.264500      26.06
 C       2.833738     0.333137    -2.812831      52.20
 H       2.283000     0.040088    -3.659231      22.84
 C       2.871145     1.819366    -0.801709      39.37
 C       2.246218     3.070257    -0.126094     107.53
 H       2.857613     4.060299    -0.563582      16.92
 O       2.580803     3.140352     1.190064     287.19
 H       3.544252     3.549053     1.279366      25.37
 C       0.629963     3.082279    -0.249488      58.26
 H       0.170303     2.818800    -1.170840      23.80
 C       0.330181     4.635779     0.064953     101.79
 O       1.241961     5.393641    -0.691262     229.08
 H       1.267800     5.202538    -1.785348      22.92
 H       0.333952     4.860991     1.267061      24.10
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 H      -0.790467     4.850208     0.020890      25.59
 C      -1.243833    -0.890804    -0.981414      17.91
 H      -0.726350    -1.947477    -0.833507      22.92
 C      -3.073723     0.286777    -0.068461      61.76
 H      -3.939864     0.253468     0.544821      21.61
 C      -2.229377     1.292736     0.321677       9.70
 O      -2.544895     2.387447     1.201212     193.36
 C      -3.910440     2.693860     1.499064     129.13
 H      -4.582220     2.701409     2.597456      24.21
 H      -4.173279     3.637526     1.130632      28.58
 H      -4.568886     1.949924     1.031583      26.43
 C      -0.830584     1.236827     0.223718      28.32
 O      -0.144821     2.260313     0.773636     186.99
 C      -0.423559     0.255265    -0.560018      42.69
 H       0.555971     0.140161    -0.783181      25.11
 C      -2.648624    -0.925764    -0.767342     -15.03
 C      -3.706126    -1.990075    -1.229419      71.95
 H      -4.716750    -1.516953    -1.345496      25.48
 O      -3.263024    -2.597947    -2.533617     224.24
 H      -4.166781    -3.027655    -2.887815      23.57
 C      -3.832901    -3.167273    -0.045642      85.67
 H      -2.820623    -3.652467     0.118400      23.69
 O      -4.386749    -2.468100     1.079825     314.94
 H      -3.737184    -2.428349     1.909187      24.49
 C      -4.702158    -4.347307    -0.445901      87.16
 O      -4.264414    -5.475551    -0.966186     277.66
 H      -4.079317    -6.118312    -0.327814      32.03
 H      -5.254322    -3.814995    -1.470245      25.44
 H      -5.495495    -4.398256     0.353639      27.37
55
name = lig-etoh-frame_240
 C       2.485374     1.411371    -2.135203      68.72
 H       1.791226     2.192469    -2.580355      23.24
 C       3.685924     1.021793    -0.203263      57.91
 H       4.065172     1.364911     0.686845      23.70
 C       4.162059    -0.261075    -0.758178      16.82
 O       5.148644    -1.223608    -0.230272     218.64
 C       5.733228    -0.863479     1.086151     115.69
 H       5.154461    -1.357502     1.988963      25.78
 H       5.907660     0.188520     1.017725      27.01
 H       6.624501    -1.533668     0.976639      26.65
 C       3.792137    -0.673623    -2.108256      20.28
 O       4.253818    -1.694951    -2.800194     173.33
 H       4.906599    -2.104354    -2.064520      20.64
 C       2.854621     0.281252    -2.835045      50.14
 H       2.191976     0.135738    -3.739531      21.64
 C       2.863158     1.924669    -0.876341      35.14
 C       2.261641     3.124291    -0.145642     115.98
 H       2.658934     3.943743    -0.538004      21.54
 O       2.613827     3.133002     1.263004     329.43
 H       3.512414     3.564033     1.332390      27.93
 C       0.561705     3.107496    -0.271768      61.53
 H       0.124351     2.762232    -1.275009      21.46
 C       0.312639     4.595628     0.139885     103.65
 O       1.313921     5.427620    -0.705864     224.37
 H       1.108918     5.314077    -1.625140      28.75
 H       0.542813     4.828077     1.110991      27.91
 H      -0.706156     4.980459    -0.091476      26.42
 C      -1.209128    -0.838851    -0.972210      61.49
 H      -0.808094    -1.823165    -1.172236      21.95
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 C      -3.167060     0.269768    -0.083480      65.68
 H      -3.932317     0.521129     0.754082      16.07
 C      -2.254522     1.261593     0.407769       6.92
 O      -2.517649     2.398509     1.231094     192.83
 C      -3.927325     2.689028     1.473261     125.08
 H      -4.466643     2.738158     2.557844      25.09
 H      -4.131987     3.783375     1.079145      25.70
 H      -4.685764     1.982950     1.120145      25.74
 C      -0.892173     1.276291     0.254251       8.08
 O      -0.053629     2.321056     0.791487     171.31
 C      -0.464287     0.251081    -0.628792      34.92
 H       0.785473     0.112923    -0.735335      21.78
 C      -2.644588    -0.884410    -0.841860      -5.78
 C      -3.696325    -2.057594    -1.177933      75.60
 H      -4.603468    -1.363873    -1.259573      23.65
 O      -3.252356    -2.599876    -2.527375     268.92
 H      -3.897758    -3.210872    -2.737951      28.87
 C      -3.745518    -3.127610    -0.033253      96.26
 H      -2.802174    -3.610739     0.278162      23.97
 O      -4.452875    -2.538542     1.096090     313.89
 H      -3.581521    -2.157187     1.660929      23.26
 C      -4.811908    -4.231226    -0.448395     101.02
 O      -4.172573    -5.487576    -0.963985     242.73
 H      -4.122058    -6.268516    -0.376164      29.83
 H      -5.417067    -3.919460    -1.169429      30.78
 H      -5.630316    -4.498575     0.273380      28.15
55
name = lig-etoh-frame_241
 C       2.523404     1.458870    -2.158612      60.81
 H       1.698179     1.943859    -2.641605      22.91
 C       3.634165     1.028761    -0.176444      66.26
 H       4.107011     1.417156     0.805919      22.65
 C       4.197862    -0.285845    -0.759750      -4.79
 O       5.206983    -1.300843    -0.249952     181.42
 C       5.689715    -0.867567     1.069996     121.98
 H       5.082890    -1.137841     1.954639      27.19
 H       6.110962     0.190669     1.251307      26.98
 H       6.636255    -1.404675     1.134380      27.94
 C       3.717737    -0.565075    -2.123748      17.66
 O       4.333540    -1.738209    -2.813754     171.73
 H       4.975996    -2.230017    -2.222392      23.33
 C       2.890816     0.200584    -2.808211      47.36
 H       2.507634     0.076359    -3.842519      23.73
 C       2.864567     1.965090    -0.940878      47.06
 C       2.257146     3.107390    -0.171247     108.69
 H       2.453284     4.194981    -0.770274      13.30
 O       2.642739     3.125349     1.338711     337.17
 H       3.452615     3.643656     1.389248      28.94
 C       0.547183     3.172235    -0.254389      74.27
 H       0.277903     2.894186    -1.242691      22.17
 C       0.306299     4.583866     0.135169      95.72
 O       1.352724     5.479733    -0.686392     105.09
 H       0.885830     5.368432    -1.661218      22.97
 H       0.822573     4.718864     1.188499      23.24
 H      -0.634095     5.008727    -0.208866      25.00
 C      -1.242674    -0.837764    -0.991863      45.11
 H      -0.743735    -1.655475    -1.644173      17.87
 C      -3.227486     0.270799    -0.055304      66.73
 H      -4.264489     0.240324     0.349532      22.08
 C      -2.283959     1.271287     0.516328       5.85
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 O      -2.545024     2.397337     1.272979     194.60
 C      -3.989350     2.723659     1.449315     118.36
 H      -3.784027     2.749838     2.641270      22.45
 H      -4.073519     3.656969     1.021689      28.20
 H      -4.675103     2.035532     0.934959      25.81
 C      -0.905226     1.305093     0.231749     -13.29
 O       0.024570     2.347349     0.791169     165.95
 C      -0.394440     0.245051    -0.653747      31.62
 H       0.555911     0.166010    -0.723450      24.20
 C      -2.666185    -0.808160    -0.861852      11.44
 C      -3.610506    -2.075658    -1.138365      83.21
 H      -4.583973    -1.601872    -1.195890      24.90
 O      -3.250281    -2.587606    -2.494904     235.72
 H      -3.670967    -3.534358    -2.652735      24.67
 C      -3.734466    -3.109364    -0.024057      93.47
 H      -2.763796    -3.507560     0.307598      23.43
 O      -4.472666    -2.581104     1.125292     332.33
 H      -3.870505    -2.079059     1.553691      33.83
 C      -4.893788    -4.166921    -0.447448      69.59
 O      -4.092886    -5.487069    -0.989843     130.02
 H      -4.147707    -6.196933    -0.182382      27.40
 H      -5.726034    -3.834598    -1.296925      25.68
 H      -5.494512    -4.551362     0.484263      26.88
55
name = lig-etoh-frame_242
 C       2.502371     1.502883    -2.254370      50.21
 H       1.633295     1.832813    -2.897585      20.51
 C       3.676977     0.967443    -0.148129      43.15
 H       3.981197     1.284348     0.857201      21.83
 C       4.202566    -0.266849    -0.778992      -6.96
 O       5.217654    -1.304385    -0.259571     175.22
 C       5.696899    -0.881002     1.058728     118.80
 H       4.861877    -0.988951     1.861805      25.83
 H       5.966161     0.144604     1.242436      27.88
 H       6.630109    -1.434107     1.381376      26.94
 C       3.762420    -0.572839    -2.091586       2.87
 O       4.391436    -1.757164    -2.816451     182.14
 H       4.997101    -2.292068    -2.345141      24.86
 C       2.882074     0.218703    -2.789715      61.81
 H       2.885902    -0.090390    -3.839694      25.76
 C       2.887768     1.934000    -0.937950      58.99
 C       2.230327     3.112908    -0.200452     115.22
 H       2.423035     3.975701    -0.605668      21.87
 O       2.657283     3.119445     1.365765     269.82
 H       3.462686     3.828175     1.407517      25.67
 C       0.629563     3.221618    -0.215395      75.37
 H       0.326128     3.001102    -1.289550      22.27
 C       0.364148     4.641476     0.108139     102.20
 O       1.333269     5.535135    -0.665008     198.30
 H       1.011789     5.525757    -1.658692      26.28
 H       0.614491     4.629836     1.161648      26.25
 H      -0.704911     5.016232    -0.030132      25.64
 C      -1.281262    -0.845136    -1.052396      43.43
 H      -0.848795    -1.343630    -1.948370      20.31
 C      -3.248108     0.276706    -0.014292      68.94
 H      -4.398190    -0.017323    -0.172317      17.74
 C      -2.313042     1.294430     0.598531       2.90
 O      -2.605222     2.384923     1.301624     179.44
 C      -3.995958     2.757994     1.462236     113.38
 H      -3.850275     2.787310     2.506106      25.68
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 H      -4.132912     3.823711     0.941205      25.72
 H      -4.649201     2.039887     0.939313      26.51
 C      -0.864881     1.292834     0.171200      -4.37
 O       0.051732     2.323364     0.770019     154.77
 C      -0.372858     0.260194    -0.607666      16.56
 H       0.875454     0.186507    -0.877904      19.49
 C      -2.695372    -0.745046    -0.827360       8.57
 C      -3.513106    -2.030589    -1.132672      78.20
 H      -4.681877    -1.884910    -1.204676      22.81
 O      -3.257759    -2.586919    -2.455554     259.31
 H      -3.203136    -3.633399    -2.388899      21.45
 C      -3.791689    -3.120315    -0.008117      69.96
 H      -2.796629    -3.586289     0.260798      21.19
 O      -4.487161    -2.611763     1.145377     245.76
 H      -3.975199    -1.858765     1.800166      22.80
 C      -4.914442    -4.181272    -0.460025      83.09
 O      -4.062076    -5.454804    -1.011824     219.27
 H      -4.006714    -5.834630    -0.166027      30.53
 H      -5.614262    -3.811137    -1.129216      29.69
 H      -5.232771    -4.412882     0.526435      28.83
55
name = lig-etoh-frame_243
 C       2.453709     1.515905    -2.363667      39.93
 H       1.770106     2.082918    -2.989878      19.80
 C       3.742785     0.889911    -0.159997      51.18
 H       3.863995     1.114229     0.904250      21.27
 C       4.218504    -0.249885    -0.779727      19.06
 O       5.198053    -1.243103    -0.262671     210.75
 C       5.698999    -0.900977     1.085784     114.52
 H       4.720497    -0.985737     1.635294      26.20
 H       5.848562     0.238202     0.957090      25.42
 H       6.436216    -1.576847     1.484073      27.08
 C       3.890805    -0.674758    -2.050779       1.77
 O       4.407812    -1.727496    -2.816651     179.41
 H       5.069187    -2.327320    -2.217081      21.32
 C       2.894448     0.267069    -2.788495      46.30
 H       3.006875    -0.128582    -3.844339      24.68
 C       2.899130     1.841694    -0.912918      36.91
 C       2.211655     3.070502    -0.168465     109.40
 H       2.770089     4.136462    -0.588150      18.65
 O       2.671216     3.129898     1.340298     283.47
 H       3.328282     3.802080     1.368354      28.65
 C       0.753622     3.225451    -0.212404      76.85
 H       0.331149     3.029901    -1.186374      22.70
 C       0.417111     4.746952     0.085496     112.71
 O       1.281437     5.601662    -0.629526     262.03
 H       1.158535     5.540090    -1.597876      29.42
 H       0.480639     4.858770     1.253365      24.96
 H      -0.650317     4.932690     0.104102      26.25
 C      -1.293142    -0.773261    -1.121710      47.01
 H      -1.032523    -1.306979    -1.983110      24.67
 C      -3.246749     0.285537     0.027499      67.69
 H      -4.294786     0.285300    -0.296719      19.80
 C      -2.323452     1.283251     0.596111      -5.19
 O      -2.662841     2.382269     1.326452     187.90
 C      -3.982541     2.817141     1.452874     120.43
 H      -4.585184     2.925364     2.654755      23.96
 H      -4.181367     3.750933     1.056841      28.08
 H      -4.672280     2.034243     1.130106      26.23
 C      -0.839965     1.285733     0.152891     -14.05
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 O       0.038104     2.270756     0.727674     156.20
 C      -0.345601     0.222450    -0.574775      52.74
 H       0.563173     0.263648    -0.950688      23.90
 C      -2.673186    -0.736246    -0.776342       9.29
 C      -3.509814    -1.972549    -1.138093      87.29
 H      -4.521335    -1.672907    -1.267589      25.05
 O      -3.235426    -2.612167    -2.413486     310.92
 H      -2.832465    -3.410407    -2.157014      26.07
 C      -3.832457    -3.133422     0.011299      74.06
 H      -2.970445    -3.746764     0.257279      19.96
 O      -4.503891    -2.611331     1.179255     285.78
 H      -3.956712    -2.016627     1.773026      25.75
 C      -4.817140    -4.233952    -0.470066      71.30
 O      -4.085164    -5.375129    -1.033489     253.72
 H      -3.583128    -5.672082    -0.147932      26.91
 H      -5.656881    -3.803666    -1.159966      26.51
 H      -5.272373    -4.449533     0.650467      26.08
55
name = lig-etoh-frame_244
 C       2.443102     1.510324    -2.384370      43.26
 H       2.009771     2.386560    -2.957886      20.72
 C       3.761763     0.872877    -0.201499      51.83
 H       3.778978     0.956874     0.956981      21.11
 C       4.293512    -0.311962    -0.773271      33.86
 O       5.177344    -1.167133    -0.262655     235.50
 C       5.633944    -0.883485     1.090228     121.31
 H       4.737792    -0.994185     1.735054      26.81
 H       6.054057     0.104907     0.961058      27.45
 H       6.349371    -1.664042     1.450624      27.07
 C       3.945083    -0.703811    -2.075668      19.08
 O       4.425612    -1.695341    -2.794944     219.15
 H       4.979200    -2.212191    -2.195181      25.40
 C       2.995557     0.245259    -2.803602      59.02
 H       2.771929     0.044367    -3.844041      24.64
 C       2.875059     1.727378    -0.905829      36.94
 C       2.312654     3.034028    -0.110931     125.48
 H       2.808041     3.772741    -0.541524      25.09
 O       2.664505     3.128343     1.283110     299.92
 H       3.379387     3.825355     1.319152      27.29
 C       0.824223     3.233116    -0.215069      47.03
 H       0.404129     3.005965    -1.219725      21.26
 C       0.445475     4.815859     0.124740      97.57
 O       1.225604     5.699613    -0.588823     198.12
 H       1.203190     5.364766    -1.654722      25.23
 H       0.649298     5.208394     1.151350      24.24
 H      -0.693671     4.859726    -0.162010      24.05
 C      -1.298986    -0.655685    -1.157069      50.90
 H      -1.091421    -1.533702    -1.924892      26.08
 C      -3.198871     0.317526     0.056372      58.71
 H      -4.308794     0.751151     0.043226      20.49
 C      -2.309329     1.261929     0.530313       2.61
 O      -2.701162     2.395705     1.369667     198.40
 C      -4.052848     2.848367     1.495098     127.04
 H      -4.663895     3.003210     2.442406      26.27
 H      -4.186131     3.886441     0.951626      26.20
 H      -4.742896     2.084908     1.109226      25.64
 C      -0.861421     1.287513     0.195215      -1.19
 O       0.014340     2.221953     0.678948     131.60
 C      -0.387831     0.158568    -0.577764      43.67
 H       0.723115     0.296689    -1.109578      20.28
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 C      -2.607881    -0.771046    -0.722045      21.13
 C      -3.568656    -1.922036    -1.128690      67.00
 H      -4.509589    -1.231859    -1.358047      21.20
 O      -3.193238    -2.639371    -2.369090     241.84
 H      -2.415886    -3.300292    -2.032176      21.86
 C      -3.860480    -3.123262     0.026247      67.10
 H      -2.932054    -3.728654     0.347647      21.30
 O      -4.521994    -2.603188     1.208172     308.39
 H      -3.765029    -2.217130     1.706951      26.25
 C      -4.729865    -4.275557    -0.452710     107.24
 O      -4.115265    -5.297211    -1.023311     292.62
 H      -3.131927    -5.490936    -0.706966      28.89
 H      -5.549037    -3.999080    -1.149433      24.85
 H      -5.340369    -4.620512     0.358969      26.56
55
name = lig-etoh-frame_245
 C       2.513931     1.472268    -2.287884      84.16
 H       2.258756     2.339251    -2.892553      24.77
 C       3.744774     0.852831    -0.232677      59.05
 H       3.808004     0.964078     0.786552      23.84
 C       4.336215    -0.353777    -0.810323      21.35
 O       5.195595    -1.133493    -0.233181     225.07
 C       5.558946    -0.872756     1.089578     127.66
 H       4.816954    -0.827713     1.995903      25.90
 H       6.229954     0.024985     1.311373      26.83
 H       6.301245    -1.658827     1.263759      27.33
 C       3.901725    -0.604071    -2.135554      35.09
 O       4.458803    -1.699102    -2.783978     229.08
 H       4.996334    -2.250798    -2.214421      26.18
 C       3.106613     0.227692    -2.843251      60.33
 H       2.621398     0.071488    -3.839796      21.43
 C       2.820831     1.642431    -0.918018      38.09
 C       2.427646     2.933506    -0.067178     105.37
 H       2.952663     3.857287    -0.818438      20.65
 O       2.667366     3.125235     1.237273     277.65
 H       3.518107     3.734611     1.355941      24.90
 C       0.840468     3.251026    -0.213779      33.34
 H       0.584830     3.080694    -1.279784      22.15
 C       0.426130     4.829241     0.174415     103.64
 O       1.190792     5.805276    -0.608168     235.98
 H       1.150560     5.456943    -1.432262      34.03
 H       0.623138     5.206074     1.162495      25.47
 H      -0.527189     4.873695    -0.286116      25.89
 C      -1.329989    -0.637897    -1.192266      57.21
 H      -0.962387    -1.492337    -1.616248      29.35
 C      -3.148231     0.349313     0.054948      55.68
 H      -4.066969     0.732890     0.555361      20.32
 C      -2.260304     1.311244     0.486606       6.74
 O      -2.721852     2.403334     1.419782     150.41
 C      -4.160694     2.879102     1.475782     108.83
 H      -4.348666     3.092657     2.731412      23.10
 H      -4.125236     3.748503     0.865661      27.10
 H      -4.826876     2.224001     0.904303      25.33
 C      -0.893292     1.251968     0.230692      14.61
 O       0.005913     2.205821     0.645728     138.37
 C      -0.388633     0.181181    -0.600725      37.66
 H       0.619865     0.214180    -0.980371      22.40
 C      -2.606210    -0.795338    -0.654934      16.28
 C      -3.641595    -1.872154    -1.110984      73.96
 H      -4.453007    -1.316805    -1.425457      23.29
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 O      -3.133098    -2.663925    -2.308267     283.84
 H      -2.278984    -3.086121    -2.079152      25.05
 C      -3.889165    -3.088019     0.042656      74.22
 H      -2.863117    -3.357443     0.335854      22.68
 O      -4.525221    -2.578278     1.234299     296.96
 H      -3.555231    -2.481518     1.811862      20.14
 C      -4.710692    -4.265923    -0.415998      85.88
 O      -4.074023    -5.293245    -1.063393     317.00
 H      -3.167401    -5.226389    -1.144005      33.16
 H      -5.480894    -3.961647    -1.266550      22.65
 H      -5.443194    -4.799004     0.375162      23.80
55
name = lig-etoh-frame_246
 C       2.643289     1.393271    -2.179041      78.11
 H       2.258505     2.139695    -2.880417      24.73
 C       3.728511     0.766674    -0.265616      63.80
 H       3.980035     1.120468     0.856677      21.19
 C       4.287971    -0.278776    -0.872277      23.37
 O       5.239232    -1.135535    -0.193209     220.15
 C       5.544353    -0.860620     1.156529     130.75
 H       4.773411    -0.795872     1.894611      27.64
 H       6.154351     0.005484     1.456851      27.97
 H       6.209197    -1.714027     1.295271      27.21
 C       3.905350    -0.551657    -2.187228      23.39
 O       4.486309    -1.715737    -2.795408     166.94
 H       5.066462    -2.332491    -2.136509      22.72
 C       3.131240     0.298923    -2.914957      70.64
 H       2.825829    -0.098859    -3.872974      21.12
 C       2.780816     1.604806    -0.882335      67.36
 C       2.477644     2.883528    -0.150883     114.50
 H       2.837535     3.616112    -0.701171      26.79
 O       2.717392     3.123614     1.245455     326.47
 H       3.555465     3.492291     1.383279      30.51
 C       0.859721     3.262378    -0.212134      45.82
 H       0.645586     3.189522    -1.281564      23.12
 C       0.423396     4.803173     0.179629      80.40
 O       1.165688     5.904705    -0.617718     163.56
 H       1.068660     5.589382    -1.659888      25.93
 H       0.327731     4.944910     1.391478      23.46
 H      -0.693812     4.934084    -0.156456      23.57
 C      -1.356316    -0.694811    -1.183365      31.64
 H      -0.716183    -1.616743    -1.569120      27.36
 C      -3.086925     0.368872     0.078327      51.06
 H      -4.051329     0.191103     0.720977      21.56
 C      -2.232201     1.427243     0.497633       7.57
 O      -2.733669     2.390686     1.452055     128.30
 C      -4.211244     2.898139     1.449698     109.35
 H      -4.268052     3.087731     2.399398      28.42
 H      -4.147785     3.883990     0.839921      25.89
 H      -4.975319     2.279137     0.931924      25.67
 C      -0.863623     1.224560     0.219264      28.93
 O       0.022820     2.232805     0.635553     146.36
 C      -0.415713     0.257703    -0.615915      26.76
 H       0.719775     0.172824    -0.866950      21.85
 C      -2.690504    -0.786145    -0.602210       1.46
 C      -3.661821    -1.878606    -1.080288      62.04
 H      -4.701643    -1.520216    -1.567099      21.07
 O      -3.082439    -2.662362    -2.243862     276.80
 H      -2.226175    -2.960516    -2.000858      24.63
 C      -3.915972    -3.009070     0.057649      77.31
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 H      -2.795842    -3.110114     0.206276      21.78
 O      -4.482524    -2.544255     1.281764     326.61
 H      -3.919348    -2.559718     1.976055      30.31
 C      -4.768591    -4.251001    -0.406103      88.40
 O      -4.009275    -5.342743    -1.137490     249.85
 H      -3.117312    -4.916737    -1.424365      26.55
 H      -5.389014    -3.702557    -1.146306      25.90
 H      -5.238998    -4.635546     0.425229      28.21
55
name = lig-etoh-frame_247
 C       2.725126     1.352358    -2.194958      57.84
 H       1.988915     2.010804    -2.750755      21.55
 C       3.693252     0.733131    -0.194892      68.10
 H       4.140515     1.044098     0.643117      24.26
 C       4.278915    -0.243150    -0.909359      14.40
 O       5.260421    -1.121870    -0.191252     191.67
 C       5.567618    -0.861045     1.255435     103.30
 H       4.456148    -0.927286     1.719794      23.92
 H       6.082589     0.136733     1.330615      26.04
 H       6.123838    -1.754577     1.687345      25.61
 C       3.986683    -0.598747    -2.241422      13.20
 O       4.505015    -1.730084    -2.809470     198.03
 H       4.984353    -2.174570    -2.127041      24.88
 C       3.145612     0.346213    -2.984242      62.32
 H       3.041967     0.004597    -4.025130      21.76
 C       2.797257     1.574321    -0.770095      58.20
 C       2.411694     2.880168    -0.215391      92.60
 H       2.998482     3.844761    -0.849925      21.30
 O       2.782279     3.098083     1.264510     276.15
 H       3.775097     3.366516     1.359340      27.33
 C       0.880982     3.262675    -0.225537      66.99
 H       0.507656     3.176453    -1.285092      22.77
 C       0.392115     4.760245     0.170410      95.29
 O       1.129734     5.957913    -0.616161     171.22
 H       0.899781     5.825564    -1.607726      27.67
 H       0.360724     4.794073     1.192608      27.72
 H      -0.641014     4.857064     0.015367      26.70
 C      -1.340933    -0.785978    -1.115269      29.14
 H      -0.822664    -1.568812    -1.589608      23.60
 C      -3.075475     0.376635     0.160123      45.70
 H      -3.904745    -0.227042     0.603099      17.06
 C      -2.259800     1.520392     0.536030       4.01
 O      -2.746935     2.372617     1.461790     149.52
 C      -4.192736     2.918127     1.342495      88.96
 H      -4.501083     3.186186     2.664718      22.61
 H      -4.215256     3.937546     0.935644      25.82
 H      -4.989578     2.203960     1.120674      24.80
 C      -0.814117     1.307612     0.198256       8.16
 O       0.068021     2.294830     0.643626     158.35
 C      -0.463969     0.276391    -0.677854      28.68
 H       0.712066     0.133715    -0.697129      21.82
 C      -2.745033    -0.754171    -0.626686       0.84
 C      -3.704700    -1.914028    -1.061661      88.48
 H      -4.614021    -1.702530    -1.499119      25.54
 O      -3.048084    -2.643482    -2.174124     234.83
 H      -2.086712    -2.903888    -1.772465      23.39
 C      -3.890568    -2.924016     0.077222      85.50
 H      -2.866179    -3.284522     0.216529      24.17
 O      -4.466934    -2.493551     1.320550     282.11
 H      -3.952571    -2.610274     2.237593      25.09
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 C      -4.770684    -4.215516    -0.447780      61.97
 O      -3.952783    -5.372856    -1.202078     176.25
 H      -3.332664    -4.687877    -1.675638      23.57
 H      -5.594819    -3.677086    -1.041870      26.85
 H      -5.157673    -4.600580     0.639707      27.85
55
name = lig-etoh-frame_248
 C       2.695470     1.392891    -2.237789      45.90
 H       1.856233     1.960356    -2.562034      20.28
 C       3.670676     0.730917    -0.079511      54.67
 H       4.304178     0.969851     0.882023      20.71
 C       4.337985    -0.303089    -0.912590       3.51
 O       5.280666    -1.104711    -0.211872     175.13
 C       5.530734    -0.874267     1.333006     106.16
 H       4.581376    -0.863795     1.655218      27.82
 H       5.947198     0.150061     1.324304      26.38
 H       6.075017    -1.597640     1.897429      27.19
 C       4.063050    -0.629613    -2.296367      20.91
 O       4.521782    -1.745449    -2.834007     206.26
 H       5.034612    -2.169145    -2.087392      22.67
 C       3.231129     0.293286    -3.024811      50.63
 H       3.110658     0.434455    -4.146974      23.79
 C       2.820680     1.556413    -0.735035      33.46
 C       2.340540     2.978977    -0.225278     114.64
 H       2.882205     3.631844    -0.750519      28.17
 O       2.850628     3.058691     1.262316     290.05
 H       3.841439     3.320271     1.181459      28.40
 C       0.872463     3.262640    -0.276567      81.49
 H       0.425946     3.029724    -1.226340      24.01
 C       0.389816     4.716243     0.119852      73.82
 O       1.065345     5.964711    -0.582270     187.61
 H       0.762792     5.864824    -1.471271      30.92
 H       0.793900     4.917393     1.298004      23.13
 H      -0.769083     4.728414    -0.090453      23.97
 C      -1.341986    -0.835782    -1.002681      31.59
 H      -0.945463    -1.669269    -1.678763      19.92
 C      -3.088088     0.334920     0.237648      33.15
 H      -4.043929     0.112555     0.801352      18.21
 C      -2.283262     1.512495     0.549973      -2.76
 O      -2.783322     2.394942     1.477063     199.40
 C      -4.156383     2.937203     1.338310     118.16
 H      -4.494517     3.124603     2.242711      28.94
 H      -4.222424     3.908729     0.791530      26.85
 H      -4.840155     2.103530     1.087324      25.35
 C      -0.826720     1.461503     0.164022     -14.22
 O       0.130671     2.370306     0.663974     166.57
 C      -0.500891     0.255491    -0.718160      24.50
 H       0.561562     0.108901    -0.780818      21.99
 C      -2.717561    -0.702375    -0.715443      11.41
 C      -3.708419    -1.936437    -1.031584      85.28
 H      -4.752005    -1.580624    -1.470622      22.82
 O      -3.002450    -2.628821    -2.094444     275.86
 H      -2.205795    -2.891982    -1.634489      25.59
 C      -3.842860    -2.915295     0.108345      76.49
 H      -2.945029    -3.556756     0.374828      21.89
 O      -4.473000    -2.421039     1.356544     285.67
 H      -3.722995    -2.708825     2.082460      23.71
 C      -4.739595    -4.180305    -0.462687      89.82
 O      -3.932612    -5.331224    -1.251385     221.60
 H      -3.598878    -4.813879    -1.950248      29.01
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 H      -5.782152    -4.041760    -0.923108      27.40
 H      -5.026676    -4.654803     0.376003      31.50
55
name = lig-etoh-frame_249
 C       2.642565     1.408529    -2.228112      45.11
 H       1.798625     2.044218    -2.688949      18.67
 C       3.726171     0.692503     0.001991      49.58
 H       4.011574     0.911163     1.022718      21.08
 C       4.383265    -0.350624    -0.848153       0.76
 O       5.323643    -1.113990    -0.225237     132.58
 C       5.468349    -0.861124     1.339822      85.59
 H       4.385107    -0.740323     1.911609      23.29
 H       5.916582     0.123645     1.508848      26.36
 H       6.209793    -1.599772     1.830096      25.20
 C       4.110824    -0.599091    -2.310581      16.63
 O       4.561758    -1.792796    -2.869829     185.91
 H       5.175171    -2.342997    -2.195363      20.73
 C       3.316899     0.288473    -3.025041      50.59
 H       3.218158     0.559841    -4.028216      24.32
 C       2.819363     1.588199    -0.797690      16.63
 C       2.312575     3.015060    -0.158670     108.07
 H       2.927765     3.854783    -0.891249      23.50
 O       2.904660     3.024482     1.224769     308.97
 H       3.737542     3.393774     1.061431      30.45
 C       0.827659     3.274838    -0.329818      88.83
 H       0.474814     2.907042    -1.342057      22.05
 C       0.423181     4.710829     0.092960     111.15
 O       0.978065     5.923325    -0.528290     182.76
 H       0.658416     5.832210    -1.591680      26.61
 H       0.830200     4.905158     0.944548      28.12
 H      -0.608291     4.697587    -0.026432      26.47
 C      -1.348893    -0.843126    -0.909329      32.66
 H      -1.043925    -1.642158    -1.608957      19.02
 C      -3.109942     0.285367     0.285642      47.04
 H      -4.027866     0.698411     0.816282      15.49
 C      -2.276782     1.446099     0.550821     -10.27
 O      -2.814084     2.445847     1.498377     182.45
 C      -4.104325     2.923060     1.311474     100.64
 H      -4.596076     3.270484     2.530681      21.90
 H      -4.164071     3.709274     0.469803      25.42
 H      -4.684035     2.136339     0.788788      24.21
 C      -0.893953     1.569484     0.097703     -11.21
 O       0.177551     2.432048     0.686180     145.47
 C      -0.523617     0.281046    -0.677131       4.82
 H       0.653745     0.097330    -1.095269      18.15
 C      -2.719149    -0.653162    -0.748611      17.24
 C      -3.670122    -1.898803    -1.004132      94.78
 H      -4.620380    -1.516625    -1.292320      24.81
 O      -2.970748    -2.626560    -2.030569     280.87
 H      -2.259605    -3.048903    -1.543823      24.82
 C      -3.845513    -2.984978     0.145555      62.94
 H      -2.948240    -3.509282     0.451348      23.59
 O      -4.452510    -2.360979     1.374221     341.69
 H      -3.721429    -2.522407     1.872570      30.04
 C      -4.694050    -4.189952    -0.482378      92.66
 O      -3.942146    -5.235774    -1.282270     217.37
 H      -3.855221    -5.018231    -2.323754      28.39
 H      -5.669144    -4.148746    -0.958694      26.27
 H      -4.889624    -4.948908     0.461741      27.44
55
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```
name = lig-etoh-frame_250
 C       2.604236     1.383881    -2.198123      64.84
 H       2.079050     2.015823    -2.878759      24.49
 C       3.754980     0.662364    -0.045821      64.36
 H       3.704334     0.884177     1.058973      20.90
 C       4.381376    -0.341992    -0.753614       7.39
 O       5.385193    -1.144529    -0.189814     150.83
 C       5.396748    -0.840286     1.328919     117.90
 H       4.574109    -0.900310     1.904496      28.89
 H       5.932751     0.119889     1.583875      26.86
 H       6.086760    -1.615871     1.510048      28.00
 C       4.169163    -0.578051    -2.263498       2.56
 O       4.615134    -1.840728    -2.906397     172.87
 H       5.197140    -2.384571    -2.443405      24.44
 C       3.361137     0.371318    -2.958730      54.25
 H       3.355124     0.307727    -4.135365      20.29
 C       2.837483     1.628581    -0.864707      23.89
 C       2.371292     3.008462    -0.131504     109.68
 H       2.690327     3.836127    -0.665447      24.41
 O       2.925671     3.002821     1.165348     290.08
 H       3.768720     3.647370     1.083758      25.51
 C       0.802106     3.282957    -0.364264      94.39
 H       0.610832     2.996285    -1.378875      23.59
 C       0.457506     4.716062     0.038803      91.56
 O       0.879132     5.868663    -0.527383     260.77
 H       0.787128     5.827143    -1.451131      32.00
 H       0.806952     4.753675     1.287316      22.30
 H      -0.735776     4.774703     0.209187      23.12
 C      -1.349240    -0.779704    -0.852702      11.81
 H      -0.968817    -1.594096    -1.429315      17.70
 C      -3.116062     0.319999     0.298175      62.34
 H      -4.115453     0.594685     0.544077      16.90
 C      -2.247494     1.400756     0.575093      -2.16
 O      -2.790196     2.476809     1.511877     189.28
 C      -4.101276     2.916599     1.281999     131.36
 H      -4.469013     3.254538     2.104418      29.73
 H      -4.051850     3.674876     0.456117      27.32
 H      -4.752508     2.206776     0.745120      26.95
 C      -0.952767     1.587626     0.033966      -1.03
 O       0.166407     2.462739     0.684814     130.41
 C      -0.490609     0.344220    -0.610918      27.96
 H       0.383604     0.299855    -1.092541      21.75
 C      -2.786464    -0.641906    -0.667784      15.81
 C      -3.577754    -1.850365    -0.952096      87.74
 H      -4.643886    -1.521628    -1.291217      23.43
 O      -2.946940    -2.629917    -1.998707     230.28
 H      -2.389724    -3.419446    -1.510189      21.46
 C      -3.891350    -3.039725     0.167711      43.29
 H      -2.822691    -3.338447     0.447484      23.43
 O      -4.431167    -2.326871     1.350788     298.63
 H      -3.546717    -2.157012     2.105716      19.18
 C      -4.641185    -4.285031    -0.457932      96.14
 O      -3.943022    -5.120426    -1.331813     300.49
 H      -4.250725    -5.154742    -2.279866      31.75
 H      -5.603694    -3.851001    -1.018821      25.33
 H      -4.768017    -4.866647     0.368452      27.35
55
name = lig-etoh-frame_252
 C       2.660107     1.363247    -2.277574      71.43
 H       2.217800     2.153243    -2.847135      24.55
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 C       3.631781     0.769805    -0.234728      57.32
 H       3.634416     0.763829     0.809178      23.72
 C       4.436140    -0.396486    -0.777105      21.81
 O       5.388661    -1.129877    -0.059962     240.43
 C       5.445006    -0.931384     1.279917     132.49
 H       4.456185    -1.083524     1.597858      27.81
 H       5.703454     0.155624     1.499745      26.73
 H       6.104774    -1.557866     1.871224      27.64
 C       4.278121    -0.595102    -2.093613      22.25
 O       4.658960    -1.761012    -2.954322     174.08
 H       5.331213    -2.338800    -2.437819      23.08
 C       3.497859     0.359165    -2.793153      50.44
 H       3.203406     0.035619    -3.868830      22.52
 C       2.935222     1.676491    -0.880625      31.22
 C       2.457769     2.950077    -0.248707     100.80
 H       2.970327     3.668333    -0.784006      22.97
 O       2.967022     3.008033     1.119424     334.60
 H       3.422351     3.810898     1.329402      29.29
 C       0.885736     3.258072    -0.316744      80.59
 H       0.534713     3.099512    -1.328704      23.58
 C       0.352497     4.637354     0.182538      72.93
 O       0.785654     5.867466    -0.603138     180.25
 H       0.777645     5.433434    -1.607069      25.87
 H       0.921742     4.743798     1.338676      21.11
 H      -0.837704     4.580453     0.192903      22.49
 C      -1.349638    -0.576092    -0.805110      66.59
 H      -0.884416    -1.439046    -1.069627      25.99
 C      -3.226433     0.473575     0.230222      53.10
 H      -4.216514     0.248794     0.574382      22.96
 C      -2.275335     1.503301     0.707957       7.66
 O      -2.666209     2.444629     1.500963     186.22
 C      -4.105360     2.962144     1.122304     106.04
 H      -4.439137     3.346519     1.962680      29.54
 H      -3.997917     3.789558     0.469920      27.54
 H      -4.790930     2.149766     0.970896      26.31
 C      -0.951794     1.551566     0.112765      18.08
 O      -0.024235     2.441466     0.559376     180.96
 C      -0.462670     0.454685    -0.547813      60.40
 H       0.449127     0.505132    -0.803558      23.33
 C      -2.659922    -0.697056    -0.368828      11.14
 C      -3.553077    -1.941337    -0.897051      76.25
 H      -4.525947    -1.547169    -1.374784      22.04
 O      -2.858567    -2.638647    -1.987504     239.48
 H      -3.156685    -3.659486    -1.891036      15.05
 C      -3.777806    -2.958548     0.222385      94.65
 H      -2.778568    -3.444057     0.505139      21.62
 O      -4.414914    -2.327241     1.301078     349.01
 H      -3.571424    -2.014148     1.907922      23.24
 C      -4.640996    -4.288655    -0.297620      82.00
 O      -3.897014    -4.956761    -1.477132     284.38
 H      -4.735514    -5.009023    -2.097172      28.74
 H      -5.664707    -3.816423    -0.742877      25.95
 H      -5.043448    -4.959971     0.406500      26.52
55
name = lig-etoh-frame_253
 C       2.768970     1.412987    -2.308377      51.12
 H       2.056077     2.058151    -2.911252      21.41
 C       3.640724     0.728763    -0.239863      59.58
 H       3.909319     0.937319     0.911210      22.08
 C       4.469410    -0.387619    -0.773702      32.82
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 O       5.367319    -1.125469    -0.064121     241.35
 C       5.471940    -0.972456     1.346055     124.10
 H       4.328416    -1.060107     1.703747      25.04
 H       5.576602     0.083355     1.573964      27.79
 H       6.244309    -1.462587     1.997178      26.55
 C       4.313529    -0.655805    -2.115051      33.80
 O       4.677240    -1.657292    -2.928338     220.98
 H       5.238876    -2.250205    -2.480493      25.96
 C       3.518931     0.268400    -2.769701      52.60
 H       3.264747     0.121210    -3.779714      23.60
 C       2.923643     1.699271    -0.957353      38.80
 C       2.474834     2.957000    -0.293236      87.99
 H       3.103124     3.743658    -1.061002      20.08
 O       2.961894     2.998437     1.130012     289.99
 H       3.412263     3.956470     1.202224      25.53
 C       0.903347     3.238513    -0.293561      68.41
 H       0.508659     3.091293    -1.325100      21.82
 C       0.326322     4.616906     0.282129      96.71
 O       0.753822     5.835357    -0.661217     224.93
 H       0.683830     5.470569    -1.480932      33.03
 H       0.705726     4.951417     1.118948      26.40
 H      -0.685761     4.477160     0.170029      25.61
 C      -1.310632    -0.560921    -0.792964      44.80
 H      -0.870128    -1.577191    -1.230255      23.29
 C      -3.259752     0.506025     0.208801      55.30
 H      -4.208841     0.548543     0.855835      21.04
 C      -2.323151     1.503959     0.678879       5.86
 O      -2.672538     2.495421     1.520010     186.13
 C      -4.065665     3.005862     1.108725      80.01
 H      -4.371922     3.507073     2.305910      22.17
 H      -4.050085     3.647760     0.091823      24.38
 H      -4.644933     2.113710     0.752721      23.40
 C      -0.962731     1.544889     0.231846      29.19
 O      -0.102766     2.449290     0.514941     154.35
 C      -0.469083     0.490858    -0.566075      37.98
 H       0.817660     0.313528    -0.669928      19.64
 C      -2.573980    -0.710367    -0.265071       9.49
 C      -3.537012    -2.017778    -0.905862      76.91
 H      -4.460369    -1.442139    -1.142263      22.74
 O      -2.806201    -2.636099    -1.988697     239.69
 H      -3.403775    -3.415689    -2.261793      16.97
 C      -3.686959    -2.961142     0.233872     108.19
 H      -2.806056    -3.463567     0.594446      21.96
 O      -4.431659    -2.331358     1.288938     355.37
 H      -3.610315    -2.264881     1.986034      23.83
 C      -4.668393    -4.186461    -0.207930      86.99
 O      -3.911568    -4.880971    -1.526177     254.26
 H      -4.613328    -5.093789    -2.202759      31.82
 H      -5.583889    -3.959374    -0.643385      27.73
 H      -4.906042    -5.130765     0.515723      25.75
55
name = lig-etoh-frame_254
 C       2.895517     1.448412    -2.349418      56.07
 H       2.123293     1.756154    -3.053377      21.60
 C       3.728524     0.661181    -0.180159      65.39
 H       3.981666     1.104760     0.683527      24.58
 C       4.468564    -0.328410    -0.725448      22.04
 O       5.378024    -1.154413    -0.073901     194.51
 C       5.432374    -0.957728     1.448064     111.50
 H       4.541497    -1.285320     2.010466      26.86
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 H       5.629594     0.128503     1.659917      26.28
 H       6.298109    -1.587216     1.730194      27.27
 C       4.302553    -0.667829    -2.156551      23.57
 O       4.724256    -1.590142    -2.916904     194.85
 H       5.275717    -2.396075    -2.473927      21.72
 C       3.464306     0.237629    -2.804932      55.60
 H       3.425543     0.022686    -3.927936      24.77
 C       2.916416     1.682799    -1.010640      50.28
 C       2.486160     2.982175    -0.306838     103.26
 H       2.780521     3.812541    -0.885726      25.46
 O       2.948060     3.013450     1.113060     326.28
 H       3.486755     3.819049     1.144417      28.97
 C       0.879078     3.240444    -0.282273      63.63
 H       0.584761     3.165446    -1.348131      22.53
 C       0.353924     4.635373     0.269776      70.98
 O       0.717088     5.775176    -0.677790     171.52
 H       0.547616     5.454885    -1.747514      24.41
 H       0.600765     5.115309     1.406173      21.69
 H      -0.819408     4.509127     0.278563      22.31
 C      -1.244164    -0.642130    -0.792711      10.87
 H      -0.924327    -1.425236    -1.377697      22.80
 C      -3.230089     0.496090     0.240775      68.97
 H      -4.129698     0.621584     0.847142      20.08
 C      -2.354937     1.482814     0.602286       7.03
 O      -2.724885     2.589222     1.538561     218.81
 C      -4.007010     3.060716     1.137272     138.54
 H      -4.380100     3.550322     1.867484      30.49
 H      -3.974389     3.559413     0.207318      28.53
 H      -4.629882     2.252125     0.814235      27.16
 C      -0.982057     1.459824     0.279978      17.04
 O      -0.117298     2.518472     0.546899     132.11
 C      -0.428792     0.509381    -0.566215      47.14
 H       0.513749     0.317693    -0.628014      23.14
 C      -2.590746    -0.716601    -0.232060       9.67
 C      -3.442777    -2.019575    -0.885912      71.01
 H      -4.439897    -1.529581    -1.039706      23.06
 O      -2.770323    -2.612194    -2.004504     271.34
 H      -3.354690    -3.211860    -2.442540      21.38
 C      -3.679037    -3.040048     0.238929      99.99
 H      -2.692687    -3.407686     0.632036      20.02
 O      -4.423811    -2.336760     1.305419     356.59
 H      -3.903851    -2.357242     2.106202      29.13
 C      -4.653432    -4.131919    -0.161492      75.04
 O      -3.949170    -4.801305    -1.548781     277.00
 H      -4.513043    -5.177039    -2.192979      34.12
 H      -5.752029    -3.820543    -0.539831      25.75
 H      -4.436388    -4.937765     0.546545      26.06
55
name = lig-etoh-frame_255
 C       2.984840     1.441438    -2.421239      52.01
 H       2.284669     1.830191    -3.182924      20.98
 C       3.776674     0.696264    -0.148149      48.49
 H       4.061073     1.253413     0.869731      19.76
 C       4.483688    -0.329617    -0.726926      14.53
 O       5.386481    -1.184373    -0.043174     155.69
 C       5.420591    -0.946678     1.519267     107.87
 H       4.627314    -1.491870     2.183978      25.51
 H       5.722382     0.073223     1.761577      26.30
 H       6.277606    -1.637432     1.499709      26.45
 C       4.230108    -0.570165    -2.114716      12.61
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 O       4.828125    -1.618749    -2.942524     196.61
 H       5.231995    -2.367210    -2.457422      24.28
 C       3.414181     0.216893    -2.904584      53.88
 H       3.488798    -0.051817    -3.951876      24.16
 C       2.963385     1.632909    -0.983650      34.92
 C       2.432827     2.974698    -0.265424      95.66
 H       2.661968     4.099539    -0.803828      22.09
 O       2.931674     3.036776     1.071785     304.38
 H       3.695055     3.664933     1.197219      28.71
 C       0.832056     3.263919    -0.265168      75.15
 H       0.587362     3.202628    -1.321245      23.44
 C       0.372487     4.709399     0.213919     110.57
 O       0.679875     5.701037    -0.694999     313.31
 H       0.500447     5.420616    -1.595472      31.19
 H       0.624999     4.873928     1.225526      26.30
 H      -0.677133     4.642032     0.356243      25.99
 C      -1.222642    -0.706766    -0.763026      25.81
 H      -0.856013    -1.474703    -1.536198      19.27
 C      -3.174055     0.428486     0.304105      44.94
 H      -4.229592     0.378692     0.642939      19.96
 C      -2.347292     1.532135     0.573725       4.48
 O      -2.763224     2.651268     1.528953     186.46
 C      -3.956105     3.094803     1.129308     109.21
 H      -4.690180     3.996805     1.854491      23.08
 H      -3.785673     3.830877     0.183817      24.33
 H      -4.814944     2.320265     1.086167      23.88
 C      -0.949855     1.413098     0.275917      12.02
 O      -0.121490     2.580169     0.631860     119.46
 C      -0.449732     0.452924    -0.549240      31.15
 H       0.821292     0.460141    -0.776227      19.01
 C      -2.618212    -0.747407    -0.304589      16.94
 C      -3.336739    -1.964072    -0.815439      78.00
 H      -4.401354    -1.740992    -1.175651      22.93
 O      -2.720743    -2.549439    -2.024733     218.01
 H      -3.373764    -3.244095    -2.489571      19.78
 C      -3.685474    -3.093693     0.257620      93.98
 H      -2.704864    -3.429495     0.600987      22.80
 O      -4.418077    -2.344505     1.309765     273.30
 H      -4.044853    -2.453926     2.374864      23.47
 C      -4.605546    -4.126134    -0.194335      89.12
 O      -3.994958    -4.706678    -1.539740     250.05
 H      -4.670145    -5.324008    -2.078590      30.39
 H      -5.570309    -3.735220    -0.157057      29.33
 H      -4.350561    -4.886300     0.628446      26.27
55
name = lig-etoh-frame_256
 C       3.000566     1.427741    -2.472854      43.71
 H       2.534606     2.277336    -3.081144      18.97
 C       3.799692     0.833630    -0.118566      44.33
 H       3.981651     1.011802     0.888326      21.09
 C       4.504967    -0.368284    -0.742836       8.84
 O       5.364320    -1.190673     0.012771     179.96
 C       5.455450    -0.985440     1.535316     109.26
 H       4.602193    -1.489905     2.119458      25.57
 H       5.705566     0.020397     1.888617      26.52
 H       6.391226    -1.588825     1.663504      26.85
 C       4.192403    -0.538987    -2.089540      13.92
 O       4.924353    -1.637133    -2.950136     156.03
 H       5.282372    -2.344989    -2.359402      23.83
 C       3.407587     0.201062    -3.009074      42.66
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 H       3.368527    -0.072802    -4.067924      23.59
 C       3.040135     1.606003    -0.952502      12.48
 C       2.355987     2.992127    -0.227780     100.45
 H       2.701238     3.850088    -0.744051      24.09
 O       2.913120     3.067178     1.049794     286.72
 H       3.908219     3.419290     1.120800      27.18
 C       0.775904     3.292772    -0.233826      70.41
 H       0.429201     3.063117    -1.299541      21.56
 C       0.377217     4.731030     0.146324      94.90
 O       0.670786     5.682313    -0.707742     274.84
 H       0.495152     5.251352    -1.685840      24.75
 H       0.992600     4.842860     1.229905      22.68
 H      -0.778538     4.689616     0.307339      22.93
 C      -1.229908    -0.757391    -0.742952      61.44
 H      -0.820299    -1.516281    -1.416220      21.33
 C      -3.123892     0.328343     0.371790      43.27
 H      -4.253128     0.151243     0.347354      18.36
 C      -2.320033     1.592376     0.604923      -7.17
 O      -2.749908     2.659455     1.509079     197.04
 C      -4.030319     3.232370     1.102266     135.24
 H      -4.301733     3.922142     1.750706      30.31
 H      -3.845277     3.750330     0.235239      29.04
 H      -4.788627     2.491743     1.160949      27.46
 C      -0.899614     1.476472     0.273194      -6.59
 O      -0.132585     2.591702     0.729398     146.33
 C      -0.408997     0.339744    -0.524813      48.60
 H       0.467164     0.657210    -0.968730      20.60
 C      -2.583448    -0.761051    -0.421206      28.22
 C      -3.310437    -1.943484    -0.768088      92.80
 H      -4.270021    -1.702756    -1.208500      24.52
 O      -2.659793    -2.473375    -2.050385     244.03
 H      -3.261905    -3.210799    -2.197298      23.23
 C      -3.635519    -3.054872     0.298872      94.94
 H      -2.731868    -3.582637     0.672978      23.95
 O      -4.421705    -2.362408     1.325447     326.73
 H      -3.962380    -2.537540     2.111651      29.23
 C      -4.516723    -4.188267    -0.246117      82.53
 O      -4.077629    -4.613971    -1.518196     302.47
 H      -4.743074    -5.307185    -1.681858      31.95
 H      -5.599044    -3.713438     0.005543      26.86
 H      -4.627039    -5.029219     0.565442      27.18
55
name = lig-etoh-frame_257
 C       2.974056     1.440446    -2.465351      48.64
 H       2.772700     2.413605    -2.833215      19.37
 C       3.860581     0.889831    -0.129311      65.57
 H       3.817289     0.871679     1.026037      20.67
 C       4.482676    -0.342607    -0.715946       2.37
 O       5.330983    -1.184971     0.076514     215.10
 C       5.520817    -1.049572     1.511311     123.55
 H       4.552957    -1.419398     1.976944      25.97
 H       5.557417     0.013890     1.895535      26.28
 H       6.415076    -1.525464     1.943224      27.54
 C       4.226383    -0.627051    -2.136259       4.69
 O       4.985212    -1.612291    -2.923134     157.15
 H       5.414359    -2.364048    -2.273022      20.39
 C       3.423232     0.227648    -3.072037      39.01
 H       3.235600    -0.084050    -4.148336      21.53
 C       3.078156     1.656385    -0.973898      11.24
 C       2.298374     2.969711    -0.213551      98.33
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 H       2.826986     3.832120    -1.022276      18.84
 O       2.898514     3.100501     1.070816     304.74
 H       3.799272     3.253583     0.885141      29.86
 C       0.712385     3.281969    -0.214194      75.72
 H       0.307383     2.932377    -1.129737      22.92
 C       0.360582     4.685853     0.178655     110.88
 O       0.689979     5.725830    -0.783586     251.29
 H       0.660031     5.294296    -1.741230      26.23
 H       1.105033     4.958469     0.896326      24.25
 H      -0.683537     4.717019     0.412553      25.23
 C      -1.195247    -0.794251    -0.752687      52.39
 H      -0.784668    -1.651404    -1.256426      21.60
 C      -3.066799     0.249928     0.387118      51.02
 H      -4.123691     0.240603     0.391919      19.42
 C      -2.295906     1.585281     0.668582     -12.22
 O      -2.721852     2.638735     1.465977     137.16
 C      -4.094396     3.353995     1.075792      77.41
 H      -3.925471     4.140035     2.095362      21.48
 H      -4.051971     3.691310    -0.107656      24.21
 H      -4.905688     2.555254     1.050920      24.33
 C      -0.884937     1.554485     0.274163      -3.86
 O      -0.129874     2.564803     0.814874     148.71
 C      -0.394660     0.305203    -0.453666      31.26
 H       0.528328     0.555567    -1.236865      19.26
 C      -2.518206    -0.717804    -0.468856      32.06
 C      -3.330063    -1.972312    -0.786826      81.03
 H      -4.360913    -1.493887    -1.093471      24.03
 O      -2.607949    -2.404581    -2.050737     236.23
 H      -3.049719    -3.281045    -2.124105      22.09
 C      -3.564543    -3.009382     0.342360      97.40
 H      -2.713016    -3.528905     0.826472      24.38
 O      -4.423616    -2.394695     1.322483     329.86
 H      -3.694252    -2.469948     2.121743      22.95
 C      -4.481565    -4.218176    -0.219700     104.65
 O      -4.183833    -4.544909    -1.504428     298.45
 H      -4.705704    -5.319011    -1.594710      32.49
 H      -5.457168    -3.833977    -0.363128      27.77
 H      -4.604206    -5.181273     0.379294      26.15
55
name = lig-etoh-frame_258
 C       2.957367     1.455659    -2.386662      41.71
 H       2.670767     2.413626    -2.965748      21.35
 C       3.929663     0.852854    -0.152106      71.68
 H       3.621224     0.934595     0.901177      20.40
 C       4.445402    -0.281530    -0.684959       1.41
 O       5.309653    -1.184271     0.109127     222.30
 C       5.545195    -1.077368     1.495504     124.37
 H       4.528629    -1.473100     1.949114      25.51
 H       5.492625    -0.020946     1.736524      26.89
 H       6.410328    -1.591514     1.991466      26.72
 C       4.288288    -0.728012    -2.214971       2.24
 O       5.021819    -1.570076    -2.860528     209.71
 H       5.470949    -2.266002    -2.438556      24.80
 C       3.461229     0.268564    -3.056215      46.56
 H       3.253603     0.008792    -4.056316      21.67
 C       3.073123     1.734122    -1.008798      24.93
 C       2.292147     2.950184    -0.264692     102.24
 H       2.560369     3.665903    -0.957346      23.28
 O       2.860448     3.136676     1.092704     286.62
 H       3.828842     3.253081     0.817941      27.71
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 C       0.675061     3.224096    -0.185563      64.63
 H       0.205759     2.889701    -1.182686      20.59
 C       0.374656     4.679628     0.191852      83.60
 O       0.717950     5.777724    -0.873386     217.12
 H       0.694159     5.434294    -1.827410      26.11
 H       1.084299     5.044562     1.071868      22.57
 H      -0.683835     4.771899     0.644549      23.20
 C      -1.103471    -0.791353    -0.766410       5.74
 H      -0.673243    -1.809552    -1.143951      21.24
 C      -2.991844     0.275081     0.372193      62.26
 H      -4.111044     0.395886     0.696768      17.79
 C      -2.264076     1.489410     0.718112      11.54
 O      -2.719754     2.618673     1.400154     141.63
 C      -4.101111     3.443979     1.054828     108.76
 H      -4.048895     4.040827     1.791173      29.54
 H      -4.163302     3.756918     0.106809      28.62
 H      -4.964648     2.810824     1.188208      27.42
 C      -0.919419     1.557961     0.281494       3.25
 O      -0.098280     2.524404     0.885838     153.56
 C      -0.351373     0.370639    -0.395340      35.22
 H       0.526294     0.177466    -1.034446      20.10
 C      -2.493356    -0.709004    -0.441820      19.43
 C      -3.349852    -1.952223    -0.848521      86.04
 H      -4.350293    -1.606546    -0.962520      25.98
 O      -2.597688    -2.368145    -2.025287     222.21
 H      -2.700332    -3.387320    -2.303652      18.53
 C      -3.534347    -3.021887     0.358768      91.04
 H      -2.576991    -3.276528     0.844056      24.09
 O      -4.392884    -2.439543     1.347859     298.29
 H      -3.723339    -1.988326     2.074198      23.32
 C      -4.484116    -4.192550    -0.131940      85.68
 O      -4.261623    -4.509087    -1.558561     241.35
 H      -4.573389    -5.476562    -1.842686      30.19
 H      -5.538552    -3.766212    -0.374481      24.22
 H      -4.350405    -5.227162     0.399098      23.94
55
name = lig-etoh-frame_259
 C       2.947504     1.490530    -2.328838      35.41
 H       2.372505     1.997914    -3.104055      21.53
 C       3.902224     0.850988    -0.196922      62.15
 H       3.711583     1.027542     0.856525      19.81
 C       4.461531    -0.300380    -0.700585      12.35
 O       5.296424    -1.197352     0.078497     211.34
 C       5.497496    -1.072976     1.503997     120.54
 H       4.657675    -1.569771     2.090962      26.34
 H       5.626179     0.030408     1.729574      25.95
 H       6.397920    -1.654826     1.724319      27.18
 C       4.287859    -0.678184    -2.220897      17.77
 O       5.069435    -1.550625    -2.837630     181.47
 H       5.580269    -2.382493    -2.396042      20.96
 C       3.536143     0.283686    -2.942939      62.51
 H       3.338882     0.173313    -4.085590      22.48
 C       3.067998     1.776516    -0.995339      41.35
 C       2.281887     2.904652    -0.303947      94.50
 H       2.430993     4.013030    -1.028778      18.61
 O       2.814931     3.170353     1.077858     274.97
 H       3.834518     3.417042     1.095658      27.19
 C       0.663557     3.152200    -0.158522      70.35
 H       0.256647     2.986687    -1.113209      21.52
 C       0.420600     4.737735     0.185020      83.19
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 O       0.743881     5.813739    -0.915150     201.85
 H       0.537923     5.391691    -1.931366      22.39
 H       0.960805     4.956283     1.155059      24.12
 H      -0.610052     4.838592     0.581608      24.27
 C      -1.034646    -0.745222    -0.736825      36.05
 H      -0.570373    -1.585950    -1.068938      25.98
 C      -2.969683     0.374886     0.372344      68.51
 H      -3.885595     0.322443     0.851078      24.72
 C      -2.231943     1.389892     0.740552      25.78
 O      -2.753908     2.613678     1.331589     150.98
 C      -4.073238     3.428537     1.036831      84.07
 H      -4.224639     4.362801     1.862785      24.09
 H      -4.080600     4.071422    -0.041699      23.48
 H      -5.015253     2.907573     1.395504      24.93
 C      -0.924450     1.495601     0.306502      13.25
 O      -0.053157     2.474192     0.928419     145.25
 C      -0.315482     0.412965    -0.358085      41.36
 H       0.863573     0.278501    -0.606719      18.68
 C      -2.471539    -0.766241    -0.399733       7.75
 C      -3.338392    -1.916987    -0.883047      78.73
 H      -4.491416    -1.754967    -1.117858      23.20
 O      -2.601541    -2.366195    -2.013754     286.84
 H      -2.652430    -3.271558    -2.223111      21.51
 C      -3.530260    -3.045392     0.346579      93.13
 H      -2.471452    -3.165863     0.677144      21.79
 O      -4.353099    -2.453504     1.390400     330.11
 H      -3.905221    -1.889015     1.930421      29.17
 C      -4.497074    -4.170940    -0.081727      85.11
 O      -4.314457    -4.490846    -1.650631     260.51
 H      -4.339703    -5.436457    -1.892716      30.15
 H      -5.478327    -3.761542     0.249160      28.56
 H      -4.316144    -4.962970     0.576127      26.97
55
name = lig-etoh-frame_260
 C       2.938571     1.481003    -2.338483      67.27
 H       2.050965     1.699984    -3.009545      19.51
 C       3.814325     0.876602    -0.233609      37.76
 H       4.077951     1.093660     0.891104      19.54
 C       4.497505    -0.360916    -0.752402      10.77
 O       5.270790    -1.214106     0.012327     203.32
 C       5.441701    -1.044396     1.499999     115.87
 H       4.748488    -1.592910     2.279549      25.22
 H       5.752265    -0.078896     1.857964      26.81
 H       6.416679    -1.596300     1.456448      26.28
 C       4.296995    -0.557748    -2.121067      26.42
 O       5.129773    -1.562840    -2.848123     188.75
 H       5.424163    -2.309087    -2.243075      23.69
 C       3.596659     0.318716    -2.831816      77.66
 H       3.546582     0.276547    -3.859225      29.18
 C       3.057024     1.794717    -0.951074      47.88
 C       2.289428     2.944995    -0.331021     125.13
 H       2.374863     3.808378    -0.787387      25.73
 O       2.767677     3.197908     1.051727     347.63
 H       3.581300     3.633261     1.218069      32.14
 C       0.696832     3.132018    -0.118935      56.33
 H       0.208399     2.952012    -1.146145      21.62
 C       0.468059     4.797293     0.151505      84.83
 O       0.759768     5.813104    -0.912607     264.13
 H       0.542651     5.369618    -1.741302      29.10
 H       1.100055     4.985140     1.044580      24.63
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 H      -0.657396     4.881139     0.280749      23.55
 C      -1.033498    -0.664645    -0.669013      37.77
 H      -0.370745    -1.517851    -1.163602      20.74
 C      -3.004005     0.358707     0.341699      54.75
 H      -4.012884     0.191500     0.879997      22.61
 C      -2.204580     1.426369     0.759259      16.00
 O      -2.806628     2.631473     1.279650     210.50
 C      -4.033957     3.422232     1.035344     122.73
 H      -4.075482     4.230906     1.686466      28.58
 H      -3.985708     3.869917     0.152586      29.00
 H      -4.931624     2.828977     1.228593      27.04
 C      -0.851267     1.426678     0.367427       4.85
 O      -0.013406     2.413877     0.934781     144.53
 C      -0.238723     0.417590    -0.341487      43.67
 H       0.781902     0.668394     0.077238      16.23
 C      -2.432906    -0.788808    -0.347229      19.92
 C      -3.348896    -1.905457    -0.879812      89.79
 H      -4.279673    -1.669255    -1.302296      24.25
 O      -2.598860    -2.372922    -2.019872     260.44
 H      -2.916192    -3.353052    -2.026555      19.10
 C      -3.529284    -3.016278     0.304460     103.94
 H      -2.519786    -3.370881     0.554739      22.25
 O      -4.337115    -2.475131     1.405420     271.83
 H      -3.698553    -1.768267     2.051276      20.26
 C      -4.492276    -4.151014    -0.070894      68.06
 O      -4.369476    -4.459994    -1.701721     236.22
 H      -4.185839    -5.396203    -1.726945      29.76
 H      -5.429138    -3.841240     0.476155      27.51
 H      -4.251826    -5.039388     0.748636      25.06
55
name = lig-etoh-frame_261
 C       2.894529     1.443839    -2.349407      59.91
 H       1.976870     1.762342    -2.797936      19.24
 C       3.787903     0.856226    -0.212096      65.91
 H       4.233726     1.131016     0.669406      25.86
 C       4.481096    -0.340485    -0.747930      28.71
 O       5.230534    -1.226261    -0.040653     210.56
 C       5.438183    -1.042821     1.473353     118.63
 H       4.707403    -1.501189     2.118356      27.19
 H       5.694553    -0.015349     1.891153      25.94
 H       6.392616    -1.530417     1.528069      28.17
 C       4.411459    -0.529418    -2.030842      23.63
 O       5.145035    -1.538354    -2.842205     223.52
 H       5.322275    -2.214506    -2.194868      26.15
 C       3.619717     0.411301    -2.773902      53.55
 H       3.712112     0.166207    -3.909812      24.58
 C       3.018103     1.791637    -0.938287      47.70
 C       2.296274     2.992834    -0.277140      99.77
 H       2.587420     4.047267    -1.060399      19.68
 O       2.707687     3.211286     1.041529     315.75
 H       3.480191     3.941532     1.080455      27.27
 C       0.742427     3.163816    -0.124726      49.33
 H       0.216795     2.852552    -1.000141      22.42
 C       0.489052     4.825476     0.102068      86.09
 O       0.787645     5.800888    -0.848709     229.01
 H       0.643774     5.321913    -1.904129      21.19
 H       1.215069     5.158163     0.982089      22.98
 H      -0.626200     4.860556     0.170876      23.22
 C      -1.016124    -0.647445    -0.625544      45.08
 H      -0.554152    -1.385969    -1.161762      22.56
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 C      -3.054477     0.281009     0.331104      46.05
 H      -4.087653     0.210061     0.605477      21.46
 C      -2.234690     1.520967     0.742586       1.88
 O      -2.826765     2.654359     1.258774     206.51
 C      -3.985077     3.350828     1.034011     108.14
 H      -3.902754     4.172622     1.848500      23.94
 H      -3.945635     3.727217    -0.189197      23.45
 H      -4.904095     2.693596     0.948656      24.75
 C      -0.795581     1.406898     0.473168       8.25
 O       0.036255     2.370022     0.929191     153.86
 C      -0.166271     0.440439    -0.260158      40.58
 H       0.858392     0.513396     0.133656      16.67
 C      -2.397598    -0.751292    -0.297822      24.00
 C      -3.317216    -1.895481    -0.846905      80.46
 H      -4.259416    -1.325774    -1.309835      21.17
 O      -2.597638    -2.429894    -2.027267     242.32
 H      -3.199363    -3.288944    -2.045772      18.03
 C      -3.550633    -2.965282     0.241513     112.57
 H      -2.635818    -3.544216     0.536686      21.64
 O      -4.302774    -2.464812     1.417424     327.64
 H      -3.590264    -2.245009     2.030345      28.16
 C      -4.469496    -4.155957    -0.056653      98.27
 O      -4.438518    -4.428022    -1.690027     225.68
 H      -3.992458    -5.374505    -1.521754      27.54
 H      -5.574103    -3.909157     0.060624      27.37
 H      -4.234626    -5.030411     0.341871      29.81
55
name = lig-etoh-frame_262
 C       2.801291     1.445942    -2.291090      41.22
 H       2.041170     2.030292    -2.903453      21.68
 C       3.798163     0.828821    -0.176851      71.35
 H       4.251661     1.277115     0.832688      22.60
 C       4.437879    -0.263443    -0.652089      33.75
 O       5.201312    -1.238484    -0.035495     229.05
 C       5.474441    -1.034101     1.417698     116.68
 H       4.437550    -1.493871     1.869557      24.81
 H       5.447814     0.028028     1.654779      26.33
 H       6.393638    -1.597554     1.787140      27.03
 C       4.531779    -0.514708    -2.093456       8.18
 O       5.119848    -1.469091    -2.805873     194.14
 H       5.438157    -2.335270    -2.224534      20.46
 C       3.683311     0.432824    -2.813313      61.14
 H       3.655354     0.095011    -3.815582      21.11
 C       2.968883     1.752226    -0.935820      34.06
 C       2.308451     3.084364    -0.263145     120.95
 H       2.662411     3.686711    -0.929577      23.40
 O       2.683756     3.244274     1.061420     337.26
 H       3.346112     3.965109     0.975830      27.66
 C       0.783346     3.229443    -0.167458      49.04
 H       0.239610     2.838540    -1.076168      20.55
 C       0.492695     4.805846     0.089632     102.95
 O       0.836652     5.791672    -0.817408     282.79
 H       0.778011     5.471549    -1.845696      24.27
 H       0.972456     5.145786     0.981785      24.92
 H      -0.613320     4.821720     0.413404      24.23
 C      -0.980439    -0.645176    -0.587753      43.74
 H      -0.679396    -1.560371    -1.257805      21.13
 C      -3.062869     0.299605     0.364955      50.63
 H      -4.192999     0.278928     0.333539      18.38
 C      -2.306313     1.540002     0.671082       1.71
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 O      -2.775564     2.657136     1.274272     229.34
 C      -3.964997     3.281343     0.947385     133.89
 H      -4.079661     4.010491     1.803094      26.03
 H      -3.931982     3.689385     0.047495      29.58
 H      -4.864875     2.660651     0.944315      27.18
 C      -0.808848     1.439769     0.593477       5.84
 O       0.118638     2.385850     0.951418     139.93
 C      -0.135383     0.413418    -0.138073      23.45
 H       1.004237     0.038475    -0.359689      17.22
 C      -2.362433    -0.720337    -0.279501      25.27
 C      -3.252989    -1.837862    -0.833739      89.38
 H      -4.121414    -1.294164    -1.016355      24.85
 O      -2.627310    -2.516589    -2.015032     270.18
 H      -3.225478    -3.202159    -2.341060      22.96
 C      -3.604576    -2.953263     0.206615     104.58
 H      -2.643297    -3.366724     0.512854      24.26
 O      -4.257199    -2.455255     1.409156     308.63
 H      -3.441131    -2.533273     2.279861      19.00
 C      -4.503836    -4.121222    -0.140861     109.41
 O      -4.492038    -4.421559    -1.634382     263.69
 H      -3.872117    -5.160813    -1.690400      29.98
 H      -5.543578    -3.950006    -0.246028      26.29
 H      -4.197093    -5.260805     0.164169      25.10
55
name = lig-etoh-frame_263
 C       2.725215     1.449580    -2.238486      65.15
 H       2.360418     2.126750    -3.007602      24.73
 C       3.805557     0.885633    -0.086303      64.20
 H       3.908402     1.234221     0.869633      23.04
 C       4.441745    -0.242403    -0.629363       7.60
 O       5.199181    -1.248331     0.006337     238.66
 C       5.450967    -1.043163     1.358920     132.98
 H       4.561874    -1.401396     1.770735      28.62
 H       5.381283     0.052280     1.476304      27.06
 H       6.239983    -1.557296     1.869360      28.33
 C       4.555654    -0.405046    -2.137667      17.42
 O       5.109465    -1.436882    -2.766626     229.70
 H       5.557284    -2.173291    -2.411321      23.20
 C       3.742730     0.413517    -2.874310      62.48
 H       3.494159     0.168175    -3.965713      20.96
 C       2.912699     1.698117    -0.898801      30.51
 C       2.301292     3.072872    -0.259385      97.55
 H       2.848859     3.968050    -1.058980      18.99
 O       2.694566     3.296601     1.102719     317.01
 H       3.437434     3.905993     1.196678      28.13
 C       0.790143     3.301790    -0.237424      60.33
 H       0.337874     2.982494    -1.184640      21.79
 C       0.448204     4.741918     0.121625      97.29
 O       0.906096     5.809746    -0.790105     229.36
 H       0.732792     5.486483    -1.806269      24.92
 H       0.897261     5.001514     1.215653      22.95
 H      -0.612322     4.806243     0.496665      24.30
 C      -0.959486    -0.675346    -0.556244      58.17
 H      -0.642898    -1.505975    -1.154776      24.04
 C      -3.053148     0.388587     0.397313      63.64
 H      -4.129504     0.396906     0.181953      19.91
 C      -2.326805     1.495916     0.601382       3.35
 O      -2.690903     2.653453     1.309939     185.70
 C      -3.992563     3.214088     0.887908     113.44
 H      -4.318875     3.977235     1.640992      26.53
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 H      -3.876444     3.969462    -0.138664      24.28
 H      -4.838928     2.493284     1.012394      25.42
 C      -0.809986     1.459712     0.662729     -19.53
 O       0.214359     2.460364     0.994671      75.88
 C      -0.140414     0.299771    -0.038187      23.86
 H       0.737799     0.184252    -0.584987      20.65
 C      -2.324989    -0.705148    -0.283943      21.03
 C      -3.188771    -1.804997    -0.828100      74.08
 H      -4.261964    -1.327026    -1.028533      23.51
 O      -2.655197    -2.584317    -1.987523     243.55
 H      -3.396183    -3.079241    -2.559494      22.59
 C      -3.634115    -2.957639     0.223919      85.01
 H      -2.570113    -3.235575     0.443361      24.40
 O      -4.197281    -2.445114     1.412923     351.86
 H      -3.666487    -2.478450     2.222589      27.86
 C      -4.549807    -4.125709    -0.297969     103.35
 O      -4.524697    -4.427723    -1.614069     275.48
 H      -3.790611    -4.953204    -1.950222      30.02
 H      -5.680700    -3.826307     0.003323      26.92
 H      -4.387061    -4.918491     0.378833      27.67
55
name = lig-etoh-frame_264
 C       2.753129     1.400709    -2.242388      59.50
 H       2.476774     2.188613    -2.972092      23.69
 C       3.787112     0.946488    -0.014101      49.59
 H       3.584660     1.133352     1.152150      18.31
 C       4.484778    -0.236743    -0.667579      -1.12
 O       5.207426    -1.254948     0.003798     210.14
 C       5.380147    -1.018538     1.339688     114.15
 H       4.462851    -1.391046     2.098524      24.86
 H       5.611370     0.060106     1.565787      26.41
 H       6.316741    -1.540775     1.724709      26.54
 C       4.524348    -0.284239    -2.097080      11.99
 O       5.111987    -1.419845    -2.765945     193.85
 H       5.711025    -2.081329    -2.243820      21.74
 C       3.702210     0.450189    -2.938018      47.85
 H       3.499983     0.333047    -4.011264      20.46
 C       2.852871     1.678891    -0.829785      43.79
 C       2.346483     3.069347    -0.289408     105.90
 H       2.667223     3.868696    -0.737090      24.19
 O       2.713463     3.348701     1.149501     274.71
 H       3.702602     3.731960     1.374488      26.22
 C       0.788434     3.352247    -0.293030      59.68
 H       0.339546     3.070996    -1.259190      22.40
 C       0.399101     4.710266     0.201094     103.80
 O       0.966388     5.819188    -0.747953     203.34
 H       0.705658     5.473398    -1.653317      28.71
 H       0.989822     4.780400     1.007756      26.53
 H      -0.723714     4.799454     0.243028      24.67
 C      -0.979711    -0.740438    -0.511108      59.25
 H      -0.425968    -1.513764    -1.105958      23.17
 C      -3.035765     0.411306     0.350057      58.41
 H      -4.102261     0.519647     0.270573      18.89
 C      -2.215349     1.521267     0.623395      -1.11
 O      -2.643983     2.668496     1.330259     161.71
 C      -4.017811     3.187587     0.832901     119.23
 H      -4.422655     3.971891     1.587778      26.32
 H      -3.913433     3.680328    -0.021972      29.63
 H      -4.678239     2.301334     0.773678      25.29
 C      -0.745273     1.423875     0.653284     -28.74
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 O       0.273621     2.540785     1.018696      31.26
 C      -0.192865     0.239610     0.062853      22.68
 H       0.808269     0.696417    -0.492825      17.45
 C      -2.336722    -0.687229    -0.290899      26.17
 C      -3.222550    -1.804373    -0.829716      80.05
 H      -4.100527    -1.439129    -1.268088      25.48
 O      -2.672394    -2.631802    -1.966742     289.55
 H      -3.522738    -2.725169    -2.398728      27.67
 C      -3.591878    -2.951156     0.252052      79.21
 H      -2.622305    -3.448836     0.418390      24.78
 O      -4.200064    -2.430344     1.381830     307.86
 H      -3.415356    -2.318419     2.326670      16.93
 C      -4.624243    -4.077580    -0.354534      94.06
 O      -4.571945    -4.457601    -1.669371     226.40
 H      -3.605810    -4.722439    -2.026955      25.37
 H      -5.498808    -3.690159     0.038917      30.09
 H      -4.471709    -4.813714     0.612600      26.19
55
name = lig-etoh-frame_265
 C       2.849725     1.363785    -2.270811      57.53
 H       2.277160     2.161053    -2.787284      21.88
 C       3.745901     0.950843     0.042228      62.01
 H       3.532578     0.870492     1.066971      20.36
 C       4.508639    -0.170590    -0.680792       3.86
 O       5.196669    -1.242332    -0.042493     217.38
 C       5.328091    -0.986666     1.424323     122.72
 H       4.599575    -1.247777     2.064309      29.46
 H       5.729647    -0.001943     1.660733      27.99
 H       6.247154    -1.568190     1.468221      27.39
 C       4.501415    -0.252697    -2.069067       3.82
 O       5.116787    -1.388853    -2.763576     153.30
 H       5.675866    -1.803130    -1.984051      21.38
 C       3.591347     0.543170    -2.947858      50.24
 H       3.669274     0.416094    -4.039588      23.75
 C       2.830784     1.683398    -0.779506      58.47
 C       2.370924     3.056864    -0.257647      94.79
 H       2.837773     4.085873    -0.915204      20.57
 O       2.744908     3.389800     1.198378     288.51
 H       3.690830     3.479267     1.156676      30.21
 C       0.798088     3.349010    -0.304440      59.61
 H       0.259880     3.020474    -1.245378      22.13
 C       0.368600     4.725460     0.223900      90.21
 O       1.012923     5.807906    -0.677643     129.39
 H       0.682078     5.491841    -1.716839      24.42
 H       1.071931     4.779865     1.203173      22.39
 H      -0.754197     4.837441     0.060676      23.35
 C      -0.982184    -0.816183    -0.454754      41.26
 H      -0.353192    -1.560260    -1.039199      22.51
 C      -2.973099     0.421856     0.255441      51.59
 H      -4.087189     0.536414     0.488498      20.27
 C      -2.050783     1.588061     0.728814      -1.60
 O      -2.637964     2.703928     1.326480     141.96
 C      -4.018196     3.131546     0.832255     104.29
 H      -4.389097     3.783870     1.564206      26.72
 H      -3.866047     3.550346    -0.383593      23.80
 H      -4.596169     2.255976     0.533367      24.70
 C      -0.669502     1.399062     0.629541       5.18
 O       0.277489     2.581892     0.997237      65.29
 C      -0.198431     0.286489     0.124925      53.44
 H       0.758243     0.576853    -0.032654      20.37
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 C      -2.411412    -0.697946    -0.316150      21.77
 C      -3.268274    -1.843703    -0.819703      80.98
 H      -4.164967    -1.347837    -1.406290      22.08
 O      -2.680758    -2.654027    -1.946444     294.98
 H      -3.517796    -2.574388    -2.408998      27.05
 C      -3.530636    -2.947272     0.232211      97.82
 H      -2.694610    -3.654377     0.451271      22.28
 O      -4.197273    -2.409793     1.394251     354.15
 H      -3.502251    -2.149764     1.906937      33.35
 C      -4.650654    -3.994028    -0.277591      75.42
 O      -4.618428    -4.506391    -1.768770     243.36
 H      -3.668716    -4.459570    -1.795040      28.40
 H      -5.742770    -3.400461    -0.270177      25.67
 H      -4.535983    -4.899111     0.306307      26.83
55
name = lig-etoh-frame_266
 C       2.859532     1.477117    -2.217684      62.10
 H       2.019999     1.995421    -2.695169      20.11
 C       3.698533     0.880091     0.027422      54.33
 H       3.652044     0.747581     1.166909      19.33
 C       4.499653    -0.070754    -0.665268      12.41
 O       5.156369    -1.186198    -0.073790     180.02
 C       5.364583    -0.965830     1.473957      92.52
 H       4.330951    -1.280346     2.127716      23.59
 H       5.706158     0.098517     1.674503      25.45
 H       6.139490    -1.755786     1.609861      26.06
 C       4.462129    -0.267481    -2.116451       7.99
 O       5.116909    -1.316330    -2.719550     202.76
 H       5.581251    -1.705637    -2.029647      25.49
 C       3.571510     0.549811    -2.934788      62.27
 H       3.802197     0.511054    -4.050580      25.38
 C       2.871216     1.683026    -0.762152      42.07
 C       2.372953     3.117119    -0.219892     104.86
 H       2.863824     3.651547    -0.891561      26.21
 O       2.762684     3.402369     1.205144     299.87
 H       3.777423     3.432679     1.055610      26.84
 C       0.812761     3.312150    -0.253612      71.55
 H       0.297401     2.941850    -1.109267      23.72
 C       0.406576     4.769981     0.195745     111.39
 O       1.035104     5.776881    -0.619746     268.85
 H       0.847183     5.640509    -1.470353      33.63
 H       0.608227     4.945650     1.195473      26.78
 H      -0.678949     4.877953     0.234779      25.67
 C      -0.958654    -0.836178    -0.369561      42.40
 H      -0.518514    -1.650486    -0.886659      22.46
 C      -2.870913     0.509191     0.202040      75.00
 H      -3.847510     0.445061     0.586125      26.10
 C      -1.982193     1.608060     0.831523       6.61
 O      -2.645613     2.747712     1.311465     189.75
 C      -3.958852     3.048949     0.759054     111.84
 H      -4.468196     3.721580     1.604443      25.46
 H      -3.839772     3.521334    -0.118232      28.50
 H      -4.681609     2.196531     0.586956      25.38
 C      -0.621071     1.508737     0.659532      22.43
 O       0.241737     2.570029     0.938971     177.95
 C      -0.174081     0.256233     0.120611      26.31
 H       1.074872    -0.009078     0.250397      18.53
 C      -2.444074    -0.741261    -0.365522       8.41
 C      -3.312681    -1.886603    -0.822967      93.42
 H      -4.234742    -1.410643    -1.070888      23.83
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 O      -2.684159    -2.652556    -1.931000     270.97
 H      -3.363723    -2.715234    -2.767376      23.81
 C      -3.543275    -2.968468     0.194379     104.73
 H      -2.643314    -3.546248     0.477714      22.60
 O      -4.214353    -2.395133     1.366479     338.60
 H      -3.416035    -1.959744     2.070131      21.52
 C      -4.719117    -3.885120    -0.242545      91.79
 O      -4.652035    -4.536720    -1.832596     209.64
 H      -3.688283    -4.376875    -1.824123      27.35
 H      -5.576526    -3.432465    -0.427901      28.69
 H      -4.695882    -4.933971     0.207601      25.37
55
name = lig-etoh-frame_267
 C       2.802240     1.642791    -2.124392      71.86
 H       1.927377     1.961904    -2.725631      19.52
 C       3.659666     0.775767     0.005014      74.54
 H       3.807155     0.905217     1.105173      21.54
 C       4.478037    -0.019762    -0.686061      25.37
 O       5.114977    -1.097027    -0.053093     214.53
 C       5.384264    -0.981808     1.488161     113.48
 H       4.484466    -1.142013     1.870196      28.16
 H       5.660223     0.024727     1.682942      27.35
 H       6.003081    -1.777836     1.932911      26.50
 C       4.396292    -0.260025    -2.156061      21.74
 O       5.117077    -1.232679    -2.675112     200.93
 H       5.631045    -1.882646    -2.035152      22.50
 C       3.625532     0.521896    -2.903172      67.89
 H       3.634375     0.567536    -3.960590      26.49
 C       2.917723     1.708722    -0.761167      37.59
 C       2.341805     3.118610    -0.148297      98.19
 H       2.977325     3.754812    -1.035036      21.05
 O       2.777642     3.391824     1.162058     309.53
 H       3.788252     3.654297     1.314129      25.88
 C       0.832794     3.292569    -0.144238      76.97
 H       0.386670     2.900787    -1.140883      22.03
 C       0.432678     4.804762     0.136724     102.66
 O       1.064558     5.765323    -0.540384     214.83
 H       0.879340     5.622286    -1.659938      23.80
 H       0.475005     5.088796     1.281578      23.91
 H      -0.747336     4.854906     0.224739      24.01
 C      -0.970815    -0.816605    -0.287650      37.53
 H      -0.577026    -1.883117    -0.645249      20.28
 C      -2.748056     0.586784     0.194631      61.37
 H      -3.818636     0.497699     0.590250      23.58
 C      -2.012224     1.583812     0.873612      14.56
 O      -2.643009     2.779256     1.299571     205.30
 C      -3.924825     2.967291     0.741051     117.05
 H      -4.414998     3.602244     1.382162      28.39
 H      -3.780945     3.772801    -0.273148      23.97
 H      -4.600299     2.141042     0.729036      25.81
 C      -0.574294     1.601438     0.676044       1.95
 O       0.211879     2.549334     0.888954     201.25
 C      -0.084973     0.176816     0.112146      29.64
 H       0.776310    -0.240249     0.254847      22.01
 C      -2.382425    -0.733472    -0.393792      16.58
 C      -3.343677    -1.913304    -0.835795      72.21
 H      -4.451785    -1.551216    -0.896532      22.66
 O      -2.688576    -2.634883    -1.950601     316.58
 H      -3.071309    -2.822826    -2.774731      28.25
 C      -3.608180    -2.998711     0.197452     101.19
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 H      -2.611586    -3.392952     0.434980      23.66
 O      -4.213301    -2.360443     1.339187     364.36
 H      -3.699503    -2.227425     2.172029      27.85
 C      -4.754446    -3.844454    -0.287623      65.77
 O      -4.670742    -4.540341    -1.851552     131.55
 H      -3.649618    -4.492254    -2.117504      25.21
 H      -5.810903    -3.219348    -0.363111      25.37
 H      -4.975248    -4.768077     0.456896      24.86
55
name = lig-etoh-frame_268
 C       2.777246     1.705250    -2.107156      52.92
 H       2.025152     2.230456    -2.708628      22.74
 C       3.613979     0.750495    -0.002396      89.85
 H       3.808357     1.053763     1.005527      24.71
 C       4.462424    -0.064034    -0.727700      26.23
 O       5.116562    -1.024086     0.001711     231.05
 C       5.384060    -0.995778     1.445094     103.36
 H       4.199823    -1.020392     1.874254      22.47
 H       5.811535     0.036915     1.770272      25.34
 H       6.016607    -1.747646     1.960895      25.18
 C       4.358706    -0.251189    -2.105563      31.97
 O       5.150510    -1.193130    -2.660847     235.88
 H       5.489769    -1.927594    -2.035661      24.53
 C       3.599165     0.610567    -2.847224      53.55
 H       3.342530     0.502560    -3.983293      20.71
 C       2.923464     1.786593    -0.736073      28.01
 C       2.376141     3.094077    -0.120136     114.18
 H       2.587219     3.938980    -0.694704      22.97
 O       2.794525     3.380371     1.145711     345.26
 H       3.627467     3.861200     1.323488      29.11
 C       0.853588     3.311580    -0.080732      87.79
 H       0.558738     3.029356    -1.048748      23.12
 C       0.382170     4.791921     0.158721     105.90
 O       1.110736     5.795025    -0.534142     242.14
 H       0.935918     5.530736    -1.445028      30.70
 H       0.701740     5.015186     1.160684      24.97
 H      -0.680992     4.802015    -0.151971      24.99
 C      -0.986468    -0.856934    -0.245532      56.46
 H      -0.564874    -1.783738    -0.309421      23.25
 C      -2.702126     0.574347     0.212739      77.05
 H      -3.748376     0.692069     0.330688      25.91
 C      -2.009141     1.573496     0.856171      13.04
 O      -2.622111     2.784144     1.297109     225.76
 C      -3.904400     2.963855     0.704187     120.71
 H      -4.476423     3.734484     1.427731      25.51
 H      -3.877443     3.435082    -0.199340      28.98
 H      -4.466228     1.987541     0.623601      24.50
 C      -0.597257     1.494405     0.628705      -9.68
 O       0.227089     2.580140     0.899377     210.94
 C      -0.066675     0.175223     0.136475      19.77
 H       1.183499    -0.088198     0.129376      18.03
 C      -2.312757    -0.654326    -0.383027      27.37
 C      -3.374303    -1.894179    -0.851639      69.07
 H      -4.379152    -1.563808    -1.121606      24.57
 O      -2.666204    -2.606437    -1.966785     296.42
 H      -3.194949    -2.767228    -2.787072      26.12
 C      -3.655751    -3.003060     0.229145      98.12
 H      -2.695534    -3.541410     0.427326      24.76
 O      -4.241883    -2.326075     1.314151     347.84
 H      -3.651870    -2.477686     2.180821      24.94
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 C      -4.833207    -3.861468    -0.381739      84.11
 O      -4.682376    -4.521966    -1.824035     235.34
 H      -3.828053    -4.661015    -2.173427      29.56
 H      -5.589003    -3.185809    -0.305762      30.38
 H      -5.096279    -4.517608     0.493672      27.57
55
name = lig-etoh-frame_269
 C       2.796085     1.690965    -2.153040      60.32
 H       2.294394     2.567613    -2.644573      23.99
 C       3.561566     0.824557    -0.026560      60.26
 H       3.803160     1.096032     1.099512      22.14
 C       4.413266    -0.130605    -0.687331      22.85
 O       5.178281    -1.002231     0.052250     262.66
 C       5.308037    -0.950107     1.418194     132.52
 H       4.462110    -0.961409     1.947172      28.89
 H       5.886348    -0.121350     1.753497      28.16
 H       5.972704    -1.827193     1.602020      26.51
 C       4.350765    -0.249270    -2.050894      21.59
 O       5.192229    -1.185705    -2.675031     251.82
 H       5.315102    -1.828463    -2.021915      28.32
 C       3.481132     0.767489    -2.799638      64.19
 H       3.253409     0.427822    -3.749290      22.77
 C       2.910645     1.876024    -0.710043      32.14
 C       2.396631     3.092035    -0.101375     105.11
 H       2.497346     4.180426    -0.720259      17.71
 O       2.806991     3.360138     1.203110     293.69
 H       3.668107     4.008678     1.088987      23.98
 C       0.885141     3.343089    -0.077564      66.85
 H       0.516214     3.072418    -1.154685      20.17
 C       0.349441     4.758249     0.205676      93.15
 O       1.161145     5.832775    -0.553776     143.00
 H       1.022071     5.550666    -1.561534      26.19
 H       0.611400     4.915602     1.272096      23.56
 H      -0.651879     4.812480    -0.362018      22.61
 C      -0.925565    -0.895286    -0.207890      30.60
 H      -0.484484    -1.991519    -0.230737      20.35
 C      -2.750264     0.531883     0.229720      63.96
 H      -3.813470     0.753667    -0.023241      18.78
 C      -1.962431     1.584231     0.798106      15.42
 O      -2.580824     2.765039     1.292863     178.14
 C      -3.926896     2.980824     0.724141     105.87
 H      -4.430174     3.620478     1.335852      27.71
 H      -3.873253     3.298106    -0.583015      23.73
 H      -4.438063     2.077133     0.576465      24.76
 C      -0.604065     1.335483     0.563509       3.17
 O       0.223970     2.586474     0.964440     127.39
 C      -0.037499     0.202977     0.183158      63.89
 H       0.937572     0.398565    -0.056112      21.25
 C      -2.311528    -0.596799    -0.356337      18.49
 C      -3.342978    -1.848740    -0.866858      62.34
 H      -4.244350    -1.365308    -1.427362      23.38
 O      -2.638418    -2.569969    -1.985598     251.85
 H      -3.506083    -2.595834    -2.596934      24.01
 C      -3.690005    -2.989105     0.210374      87.74
 H      -2.914657    -3.710705     0.472609      24.39
 O      -4.279383    -2.296536     1.317103     329.85
 H      -3.548453    -2.565052     2.072666      23.01
 C      -4.860137    -3.901343    -0.488393      78.41
 O      -4.731758    -4.490225    -1.753039     258.50
 H      -3.792259    -4.754334    -1.927736      28.85
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 H      -5.693333    -3.018414    -0.599784      26.75
 H      -5.208505    -4.629061     0.427827      26.79
55
name = lig-etoh-frame_270
 C       2.781104     1.775267    -2.138711      61.13
 H       2.554379     2.682584    -2.693190      24.88
 C       3.545453     0.940838    -0.017399      54.78
 H       3.677293     0.999050     0.988789      23.25
 C       4.316377    -0.163129    -0.593594      12.30
 O       5.244238    -0.998643     0.045787     217.17
 C       5.285937    -0.916121     1.426469     116.68
 H       4.322379    -0.997868     2.213411      24.25
 H       6.013722    -0.076649     1.758143      25.92
 H       5.793229    -1.905033     1.427392      25.47
 C       4.329080    -0.213766    -2.041989       6.47
 O       5.209313    -1.165489    -2.699701     199.21
 H       5.285112    -1.931856    -1.963637      22.78
 C       3.433515     0.782928    -2.763867      62.48
 H       3.241840     0.478489    -3.860302      21.18
 C       2.909820     1.916694    -0.733935      36.15
 C       2.375440     3.191850    -0.092777     118.83
 H       2.797852     3.886318    -0.770059      23.70
 O       2.834435     3.354291     1.284557     308.53
 H       3.682645     3.759372     1.193865      28.10
 C       0.879581     3.336727    -0.120760      72.91
 H       0.446588     3.051059    -1.028018      23.78
 C       0.368473     4.751881     0.207025      96.53
 O       1.194344     5.846937    -0.574017     140.78
 H       1.088426     5.644661    -1.641286      25.46
 H       0.170306     4.969496     1.330026      24.23
 H      -0.642745     4.841384    -0.074967      25.85
 C      -0.835027    -0.935381    -0.172040      42.92
 H      -0.609148    -1.907153    -0.459609      20.75
 C      -2.863261     0.548189     0.237536      64.44
 H      -3.840938     0.710792    -0.220456      18.23
 C      -1.965976     1.568338     0.709916      11.82
 O      -2.536090     2.733982     1.271794     166.14
 C      -3.919290     2.996789     0.681524     111.15
 H      -4.477150     3.789034     1.348724      25.91
 H      -3.805229     3.217417    -0.269295      29.73
 H      -4.617389     2.072521     0.766681      23.85
 C      -0.604947     1.344787     0.569343      13.60
 O       0.197036     2.539819     1.030090     111.84
 C      -0.027485     0.168726     0.183133      49.47
 H       1.076138     0.482981    -0.185059      19.28
 C      -2.294319    -0.660736    -0.323534       9.33
 C      -3.245850    -1.780746    -0.872096      80.54
 H      -4.039408    -1.190684    -1.367971      24.54
 O      -2.643939    -2.521629    -2.003406     309.79
 H      -3.428573    -2.646807    -2.481350      28.19
 C      -3.762227    -2.953257     0.129903      77.51
 H      -2.974756    -3.677698     0.484606      23.31
 O      -4.301909    -2.294722     1.332695     369.52
 H      -3.698350    -2.268414     2.044824      29.85
 C      -4.920644    -3.866600    -0.525559     106.65
 O      -4.765178    -4.473877    -1.706626     256.51
 H      -3.809735    -4.879979    -1.552191      28.26
 H      -5.707283    -3.263716    -0.855549      28.15
 H      -5.263961    -4.684062     0.151742      27.39
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name = lig-etoh-frame_271
 C       2.768149     1.921154    -2.100289      58.84
 H       2.513505     2.708883    -2.826123      21.37
 C       3.582540     0.995520     0.009315      53.33
 H       3.469285     1.035370     1.210883      17.79
 C       4.210531    -0.144179    -0.562426       4.26
 O       5.258900    -0.971399    -0.004970     194.23
 C       5.307159    -0.925341     1.507458     120.34
 H       4.383763    -0.920581     1.944079      28.48
 H       5.937583    -0.134205     1.780168      28.04
 H       5.716677    -1.907921     1.833185      27.10
 C       4.288055    -0.169835    -2.032689       3.48
 O       5.184442    -1.129522    -2.698201     199.31
 H       5.392404    -1.945270    -2.173623      23.35
 C       3.459258     0.659868    -2.775599      40.82
 H       3.385401     0.758346    -3.842492      23.99
 C       2.890717     1.954884    -0.763989      37.79
 C       2.379963     3.270588    -0.063959      98.56
 H       3.070894     3.954055    -0.796929      21.15
 O       2.834849     3.345402     1.351022     262.18
 H       3.927400     3.578504     1.489484      25.02
 C       0.832982     3.334171    -0.113752      44.66
 H       0.366915     2.902860    -1.077791      21.97
 C       0.389257     4.789053     0.183566     104.15
 O       1.199288     5.832572    -0.583617     195.67
 H       1.022667     5.636020    -1.439989      32.61
 H       0.236472     5.066491     1.198265      26.64
 H      -0.781043     4.854021    -0.007508      25.14
 C      -0.821167    -0.947218    -0.160440      47.08
 H      -0.466038    -1.891066    -0.750114      18.70
 C      -2.936827     0.529783     0.184801      52.18
 H      -3.952154     0.732861    -0.125846      18.06
 C      -2.046062     1.539130     0.623530       5.57
 O      -2.508748     2.704318     1.231384     161.25
 C      -3.918534     2.991516     0.721574     102.28
 H      -4.215621     3.939280     1.173754      27.15
 H      -3.736479     3.376201    -0.523512      23.73
 H      -4.614046     2.241997     1.009883      25.86
 C      -0.595720     1.456268     0.629508       5.91
 O       0.172327     2.465364     1.064917     158.67
 C       0.018651     0.127544     0.137100      18.26
 H       1.111165     0.025093    -0.071021      19.64
 C      -2.237334    -0.753902    -0.243527      30.26
 C      -3.135298    -1.720942    -0.864498      81.25
 H      -4.054361    -1.086021    -1.143964      23.63
 O      -2.647165    -2.465327    -2.012401     279.92
 H      -3.354351    -2.894572    -2.592718      24.84
 C      -3.841780    -2.892423     0.071254      76.70
 H      -2.952367    -3.472968     0.305258      23.26
 O      -4.348733    -2.308060     1.323737     310.67
 H      -3.619391    -1.923485     2.083230      22.68
 C      -5.019962    -3.759101    -0.489466      88.93
 O      -4.726306    -4.504707    -1.728081     267.83
 H      -4.028422    -5.093534    -1.532346      31.98
 H      -6.023450    -3.189875    -0.724516      26.29
 H      -5.351769    -4.650448     0.281097      25.36
55
name = lig-etoh-frame_272
 C       2.821974     1.960559    -2.144196      32.86
 H       2.288652     2.683854    -2.823031      20.71
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 C       3.611903     1.000455     0.080033      60.59
 H       3.388820     1.169520     1.043747      21.15
 C       4.162063    -0.098007    -0.572548       5.14
 O       5.234645    -0.934055    -0.031779     150.29
 C       5.346027    -0.970166     1.554170      93.21
 H       4.159854    -0.731853     1.774378      23.07
 H       5.933810    -0.026237     1.900517      25.36
 H       5.741074    -1.813455     2.166433      26.00
 C       4.257931    -0.184329    -2.017223      10.18
 O       5.127517    -1.067793    -2.689660     222.29
 H       5.410027    -1.848347    -2.246999      25.45
 C       3.454822     0.625501    -2.777297      51.70
 H       3.642165     0.817064    -3.859547      25.06
 C       2.861915     2.021378    -0.736808      31.30
 C       2.446612     3.298826    -0.026514     106.64
 H       2.838000     4.232261    -0.472348      23.95
 O       2.824758     3.339278     1.405906     332.35
 H       3.776215     3.495146     1.521270      29.53
 C       0.783353     3.354022    -0.072690      34.97
 H       0.472323     2.869958    -0.974299      23.62
 C       0.357911     4.848674     0.137887     102.36
 O       1.175760     5.793108    -0.563537     129.84
 H       0.853552     5.544471    -1.626004      24.83
 H       0.757569     5.133728     1.246338      23.84
 H      -0.622493     4.907686    -0.202313      26.81
 C      -0.838526    -0.957559    -0.190988      46.59
 H      -0.295537    -1.667157    -0.772642      20.95
 C      -2.918425     0.448075     0.096705      53.63
 H      -4.034988     0.641468     0.108113      22.53
 C      -2.108587     1.515711     0.568519      -2.79
 O      -2.522776     2.684708     1.171020     199.80
 C      -3.859961     3.046281     0.741315     123.52
 H      -3.960016     4.086079     1.145904      26.98
 H      -3.954051     3.122293    -0.284724      29.23
 H      -4.644427     2.317718     1.112593      26.47
 C      -0.591702     1.447980     0.648587      -2.26
 O       0.179775     2.429116     1.084406     167.50
 C       0.033114     0.144525     0.116700       3.48
 H       1.137061    -0.253106     0.100939      19.35
 C      -2.197523    -0.792431    -0.140556      42.07
 C      -3.137091    -1.709660    -0.874068      84.06
 H      -4.030795    -1.066802    -1.040694      23.96
 O      -2.633602    -2.394013    -2.031461     245.01
 H      -3.260760    -3.174009    -2.414565      21.44
 C      -3.887515    -2.800257     0.060716      86.59
 H      -2.992346    -3.498516     0.131428      22.26
 O      -4.401191    -2.311487     1.318122     342.85
 H      -3.605131    -1.972931     1.700941      27.96
 C      -5.132703    -3.663718    -0.444136      78.23
 O      -4.684665    -4.526469    -1.763563     190.93
 H      -4.154285    -5.336923    -1.494699      28.94
 H      -6.046394    -3.082464    -0.508481      28.43
 H      -5.323083    -4.283244     0.443049      27.90
55
name = lig-etoh-frame_273
 C       2.902301     1.896131    -2.198097      45.95
 H       2.212644     2.545109    -2.707132      20.68
 C       3.580034     1.033800     0.085922      46.04
 H       3.502841     1.236856     1.264340      17.81
 C       4.196669    -0.064097    -0.574261      10.04
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 O       5.205200    -0.912606    -0.014454     191.94
 C       5.326148    -0.951628     1.573007     115.60
 H       4.334761    -0.715080     1.806855      26.63
 H       5.852120    -0.082577     1.857745      28.20
 H       5.727139    -1.840132     2.060771      27.63
 C       4.221513    -0.227174    -1.994757       9.74
 O       5.053985    -0.993061    -2.686874     186.65
 H       5.402113    -1.790962    -2.057443      22.10
 C       3.423961     0.723952    -2.782197      68.72
 H       3.809813     0.598423    -3.825290      25.30
 C       2.884353     2.072495    -0.709724      41.53
 C       2.463434     3.307689     0.055748     108.55
 H       2.628829     4.424655    -0.327217      21.27
 O       2.779042     3.319907     1.449920     296.71
 H       3.795420     3.645614     1.433183      26.17
 C       0.786068     3.377831     0.004034      48.85
 H       0.497751     2.908052    -0.974734      22.46
 C       0.361824     4.888590     0.149780     113.96
 O       1.133206     5.744365    -0.608946     189.85
 H       0.943537     5.672711    -1.538506      30.08
 H       0.745382     5.031473     1.076560      27.28
 H      -0.756929     5.096417    -0.180403      25.24
 C      -0.815498    -0.913780    -0.228302      46.42
 H      -0.310304    -1.766839    -0.717446      20.76
 C      -2.844461     0.390527     0.053844      69.89
 H      -3.889114     0.327598     0.245239      27.31
 C      -2.088120     1.484640     0.542172       2.03
 O      -2.554280     2.667169     1.093018     194.36
 C      -3.811517     3.112946     0.805186     108.18
 H      -3.850029     4.194853     1.171127      25.45
 H      -4.115652     2.915587    -0.502219      23.93
 H      -4.631968     2.533485     1.259672      26.76
 C      -0.610919     1.308538     0.603790       6.18
 O       0.216001     2.448957     1.095920     149.14
 C      -0.004263     0.192639     0.133637      43.36
 H       1.103495    -0.092506     0.339332      19.47
 C      -2.224744    -0.822456    -0.095449      40.96
 C      -3.234640    -1.735650    -0.871780      76.87
 H      -4.019914    -1.019001    -1.298110      22.34
 O      -2.619708    -2.331699    -2.050176     274.88
 H      -3.091403    -3.137282    -2.007558      23.94
 C      -3.911628    -2.747329     0.040444     109.44
 H      -3.248195    -3.614625     0.196706      20.62
 O      -4.440497    -2.307615     1.294540     322.76
 H      -3.573195    -2.001472     1.719174      23.77
 C      -5.171531    -3.585491    -0.429239      53.99
 O      -4.665831    -4.519000    -1.769015     141.31
 H      -4.395303    -5.394363    -1.276158      28.40
 H      -6.063300    -2.936261    -0.685276      27.04
 H      -5.273328    -4.157566     0.656442      25.55
55
name = lig-etoh-frame_274
 C       2.945073     1.838568    -2.177859      63.46
 H       2.260005     2.515634    -2.776138      23.43
 C       3.513511     1.096822     0.077436      73.49
 H       3.809823     1.147897     1.085794      23.95
 C       4.268398    -0.037207    -0.563113      19.06
 O       5.182311    -0.910075     0.048780     211.42
 C       5.285725    -0.902356     1.533603     103.07
 H       4.194847    -0.811539     2.102336      23.53
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 H       5.991961    -0.038022     1.817179      25.39
 H       5.698815    -1.952020     1.682950      25.31
 C       4.121742    -0.188518    -1.959190      27.68
 O       4.999885    -0.965871    -2.681854     225.39
 H       5.367927    -1.548346    -2.016941      26.81
 C       3.459105     0.795608    -2.780367      54.65
 H       3.579043     0.528305    -3.817061      22.16
 C       2.971979     2.077483    -0.706053      30.73
 C       2.384463     3.326357     0.137578     108.62
 H       2.662350     4.295189    -0.413068      20.47
 O       2.758120     3.297581     1.493274     312.62
 H       3.626301     3.903496     1.517628      24.30
 C       0.809971     3.365248     0.070018      70.74
 H       0.488720     3.055198    -0.947315      21.51
 C       0.330485     4.878255     0.168954     104.82
 O       1.117416     5.735551    -0.680506     217.67
 H       0.907154     5.604007    -1.690751      24.85
 H       0.450120     5.151665     1.380060      24.03
 H      -0.703355     5.116615     0.224591      26.42
 C      -0.798715    -0.880856    -0.273699      54.74
 H      -0.466221    -1.933812    -0.510980      24.07
 C      -2.772282     0.391365     0.090938      70.21
 H      -3.874173     0.205786     0.267304      22.99
 C      -2.016806     1.449391     0.532396      18.04
 O      -2.546295     2.639456     1.014991     227.95
 C      -3.827498     3.181937     0.808934     130.38
 H      -3.828439     4.221893     1.045022      27.49
 H      -4.117725     2.976564    -0.104946      29.90
 H      -4.603227     2.728607     1.514584      26.71
 C      -0.653282     1.272620     0.570769      12.09
 O       0.240824     2.469416     1.088984     119.00
 C      -0.026253     0.177502     0.166789      58.24
 H       1.041740     0.276608     0.363543      19.48
 C      -2.244726    -0.881121    -0.144893      32.09
 C      -3.339080    -1.733410    -0.869435      80.06
 H      -3.972890    -1.055250    -1.490542      21.54
 O      -2.626699    -2.284644    -2.036267     237.98
 H      -2.832740    -3.323021    -1.894621      18.27
 C      -3.964005    -2.772119     0.008097     115.80
 H      -3.292679    -3.607629     0.327926      20.29
 O      -4.447999    -2.272095     1.273725     314.01
 H      -3.755348    -2.064442     2.094585      23.60
 C      -5.162179    -3.520779    -0.438787      92.29
 O      -4.672413    -4.490988    -1.712539     206.29
 H      -4.619659    -5.253591    -1.189067      31.88
 H      -5.967132    -2.975771    -1.030845      27.23
 H      -5.440501    -4.149919     0.346518      29.54
55
name = lig-etoh-frame_275
 C       2.905180     1.892149    -2.099261      69.28
 H       2.476124     2.562109    -2.802852      26.33
 C       3.531059     1.075622     0.055997      69.63
 H       3.907340     1.262038     1.106224      22.55
 C       4.297786     0.025457    -0.552716       7.77
 O       5.141734    -0.901736     0.120622     240.67
 C       5.229966    -0.858576     1.479319     136.17
 H       4.460734    -0.965741     2.213781      27.63
 H       6.020674    -0.204049     1.816313      27.67
 H       5.691145    -1.831118     1.473723      26.36
 C       4.050980    -0.119755    -1.926541      36.00
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 O       4.948298    -0.967244    -2.672741     211.49
 H       5.457489    -1.499023    -2.047764      27.01
 C       3.538359     0.779567    -2.781861      34.39
 H       3.154878     0.647592    -3.867582      18.83
 C       3.037136     2.100210    -0.713964      29.17
 C       2.287632     3.313130     0.161437     109.50
 H       2.780390     4.182915    -0.446003      20.40
 O       2.754924     3.297693     1.543043     324.96
 H       3.464340     3.886999     1.690431      28.71
 C       0.816000     3.355919     0.110670      76.07
 H       0.525171     3.091419    -0.904012      20.51
 C       0.309316     4.859781     0.274004      97.28
 O       1.095580     5.747720    -0.751257     183.86
 H       0.744006     5.268632    -1.683324      22.92
 H       0.428872     5.301539     1.174288      26.35
 H      -0.857421     4.933870     0.242128      24.25
 C      -0.824357    -0.944123    -0.313141      62.05
 H      -0.395473    -1.908988    -0.377147      24.59
 C      -2.759818     0.362503     0.171039      48.06
 H      -3.829058     0.549684     0.224648      22.84
 C      -1.996371     1.456007     0.540232      27.38
 O      -2.500361     2.628868     0.953974     193.34
 C      -3.872049     3.220219     0.855448      93.41
 H      -3.685729     4.412783     0.836550      23.95
 H      -4.385480     3.019339    -0.361102      22.81
 H      -4.480594     2.926122     1.738100      25.21
 C      -0.649961     1.387371     0.575810       5.48
 O       0.235399     2.460688     1.068960     168.43
 C      -0.011995     0.110643     0.197975      22.08
 H       1.153996     0.471453     0.160288      17.37
 C      -2.241665    -0.886469    -0.247124      31.38
 C      -3.373239    -1.717187    -0.898362      75.24
 H      -4.163966    -1.043968    -1.304301      23.69
 O      -2.660533    -2.295445    -1.996204     289.66
 H      -2.435923    -3.242607    -2.116938      22.89
 C      -4.002248    -2.827118     0.039306      97.19
 H      -3.125329    -3.466375     0.238334      22.78
 O      -4.461917    -2.205168     1.288826     340.04
 H      -3.919205    -2.257522     2.001410      31.17
 C      -5.151862    -3.493230    -0.558495     102.97
 O      -4.693057    -4.437584    -1.613871     232.00
 H      -4.701528    -5.329523    -1.158388      30.02
 H      -5.858177    -2.939677    -1.102957      28.75
 H      -5.893379    -4.264036     0.096630      24.96
55
name = lig-etoh-frame_276
 C       2.873013     1.960364    -2.053414      66.71
 H       2.548939     2.814735    -2.735800      25.29
 C       3.637905     1.023059     0.081005      70.23
 H       3.681721     1.443231     1.120290      21.18
 C       4.285603     0.095657    -0.533284      30.65
 O       5.056039    -0.865910     0.115991     251.07
 C       5.248340    -0.871818     1.478470     119.01
 H       4.308904    -0.930639     2.204912      25.18
 H       6.012766    -0.131516     1.874143      26.16
 H       5.826364    -1.845778     1.709785      25.64
 C       4.105769    -0.124174    -1.929785      26.44
 O       4.886717    -0.990443    -2.652942     194.97
 H       5.577595    -1.559271    -2.076589      24.77
 C       3.510020     0.836010    -2.774243      51.24
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 H       3.087667     0.698768    -3.712839      21.16
 C       3.023686     2.146977    -0.695838      30.62
 C       2.293067     3.272690     0.153616     104.28
 H       2.772995     4.239869    -0.338102      20.41
 O       2.726590     3.291980     1.587017     263.99
 H       3.630501     3.944843     1.713906      22.74
 C       0.790149     3.380620     0.129618      57.40
 H       0.512620     3.044615    -0.932697      20.02
 C       0.282280     4.850550     0.349580      89.19
 O       1.023075     5.723493    -0.797550     145.75
 H       0.816235     5.305765    -1.631330      27.25
 H       0.713260     5.497341     1.285899      21.69
 H      -0.707267     4.688413    -0.059649      23.15
 C      -0.837496    -1.029012    -0.319674      40.83
 H      -0.213331    -1.967778    -0.474849      22.62
 C      -2.780306     0.331083     0.252488      53.73
 H      -3.797629     0.778756     0.143438      19.53
 C      -2.018181     1.476305     0.559848      13.86
 O      -2.481927     2.682712     0.911406     186.82
 C      -3.892510     3.261606     0.841269     125.12
 H      -3.602720     4.226480     0.735171      28.17
 H      -4.519396     3.029802     0.093115      29.05
 H      -4.406541     3.063668     1.783139      27.34
 C      -0.541990     1.461338     0.573605      11.11
 O       0.203134     2.429939     1.053089     214.66
 C      -0.005485     0.123282     0.219585      19.28
 H       1.026172     0.046297    -0.018141      22.23
 C      -2.268827    -0.819564    -0.343563      28.82
 C      -3.360643    -1.733022    -0.914410      70.23
 H      -4.308899    -1.103157    -1.049725      24.02
 O      -2.694136    -2.314836    -1.997514     311.38
 H      -2.411441    -3.195156    -2.057371      25.49
 C      -3.993522    -2.839309     0.123403      72.70
 H      -3.085197    -3.483279     0.180263      25.14
 O      -4.498874    -2.134345     1.289998     311.47
 H      -3.729212    -2.455230     1.989798      23.60
 C      -5.210213    -3.550269    -0.700933      97.01
 O      -4.707649    -4.399558    -1.523852     253.43
 H      -4.663697    -5.375825    -1.224442      30.17
 H      -5.795550    -2.571482    -1.150429      27.55
 H      -5.916202    -3.914820    -0.063501      28.38
55
name = lig-etoh-frame_277
 C       2.869014     2.041809    -2.057632      39.05
 H       2.474073     2.916968    -2.520094      24.48
 C       3.674162     1.139462     0.147254      61.13
 H       3.586106     1.275696     1.196979      22.03
 C       4.302866     0.082429    -0.542446      29.88
 O       4.977009    -0.851923     0.073316     218.42
 C       5.300797    -0.914476     1.558856     113.97
 H       4.256512    -0.755874     1.885159      25.60
 H       5.778195     0.064521     1.811288      26.92
 H       5.809593    -1.778615     1.901557      27.32
 C       4.203024    -0.108109    -1.976610      27.72
 O       4.843823    -1.053686    -2.636507     251.07
 H       5.438676    -1.536322    -2.086254      27.02
 C       3.414147     0.932647    -2.695233     106.69
 H       3.253856     0.644530    -3.823576      19.48
 C       2.977914     2.144170    -0.622299      45.37
 C       2.375729     3.247091     0.154059     106.14
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 H       2.631020     4.320891    -0.247179      19.63
 O       2.712389     3.302258     1.620186     304.81
 H       3.557298     3.677888     1.521453      28.96
 C       0.781773     3.407725     0.121984      62.47
 H       0.434938     3.128188    -0.835971      21.65
 C       0.310457     4.856711     0.349141     104.59
 O       0.932466     5.692496    -0.777330     184.07
 H       0.828290     5.355928    -1.878347      20.94
 H       0.593019     5.324636     1.229792      25.91
 H      -0.746069     4.806239     0.037873      24.67
 C      -0.847451    -1.036468    -0.282127      26.69
 H      -0.385363    -1.884180    -0.745384      19.14
 C      -2.808658     0.375397     0.315819      56.48
 H      -3.875190     0.571260     0.053936      18.66
 C      -1.985046     1.479026     0.590422       2.43
 O      -2.495951     2.778351     0.876095     161.42
 C      -3.863432     3.275988     0.863454      94.74
 H      -3.596379     4.449783     0.648277      23.76
 H      -4.783888     2.778228     0.052694      22.97
 H      -4.341335     3.195837     1.921727      25.02
 C      -0.488030     1.388844     0.538971      31.06
 O       0.192099     2.437889     1.064393     204.40
 C      -0.038883     0.139055     0.200218      41.17
 H       0.996043    -0.446743    -0.022349      18.36
 C      -2.295512    -0.763069    -0.404271      15.96
 C      -3.335736    -1.762455    -0.864881      86.26
 H      -4.223212    -1.208277    -1.169857      25.16
 O      -2.732554    -2.332329    -2.054679     266.86
 H      -2.671922    -3.350360    -1.749965      22.64
 C      -3.985674    -2.818830     0.159940      79.58
 H      -3.283162    -3.653195     0.442338      25.29
 O      -4.504704    -2.095442     1.299913     335.04
 H      -3.754581    -2.289669     1.987942      25.91
 C      -5.282167    -3.475194    -0.740127      80.98
 O      -4.689918    -4.440392    -1.533742     271.76
 H      -4.647354    -5.284637    -1.146736      34.36
 H      -5.550762    -2.653468    -1.287907      31.20
 H      -6.091517    -3.703488     0.158697      27.02
55
name = lig-etoh-frame_278
 C       2.873996     2.128892    -2.016648      52.89
 H       2.285098     2.947083    -2.514037      19.74
 C       3.677164     1.286007     0.184241      57.90
 H       3.632965     0.998560     1.304191      20.63
 C       4.294485     0.097038    -0.572783       1.08
 O       4.968526    -0.921934     0.059797     181.03
 C       5.294826    -0.881106     1.596665     108.38
 H       4.261803    -0.786953     1.968505      25.47
 H       5.700154     0.107741     1.763533      26.59
 H       5.818784    -1.838511     1.920107      25.98
 C       4.244102     0.010720    -1.994402      11.21
 O       4.811438    -1.142163    -2.650016     217.02
 H       5.326597    -1.608638    -1.955374      23.85
 C       3.346744     0.962634    -2.638479      69.01
 H       3.494829     0.840921    -3.684439      26.07
 C       2.946284     2.113063    -0.549914      41.35
 C       2.411311     3.276540     0.183603     103.02
 H       2.618240     4.345766    -0.259894      22.71
 O       2.700267     3.307598     1.618515     265.89
 H       3.728927     3.546292     1.569313      25.81
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 C       0.808380     3.407144     0.115801      62.17
 H       0.357590     3.170984    -0.928653      20.63
 C       0.327411     4.850843     0.256431     111.45
 O       0.852919     5.671461    -0.748090     286.26
 H       0.578502     5.360531    -1.569470      31.33
 H       0.513300     5.266338     1.371448      24.08
 H      -0.791853     5.030893     0.460612      24.91
 C      -0.927163    -0.954957    -0.249931      52.86
 H      -0.576188    -1.784435    -0.924001      19.31
 C      -2.836739     0.438035     0.315238      38.40
 H      -3.914311     0.392310     0.219325      17.47
 C      -1.948986     1.496882     0.624256      -0.23
 O      -2.495073     2.862505     0.839383     190.49
 C      -3.852342     3.302516     0.877286     134.59
 H      -3.919628     4.267043     0.556050      29.20
 H      -4.431668     2.704809     0.314173      29.01
 H      -4.194092     3.288529     1.882668      28.45
 C      -0.526074     1.293606     0.518883       9.97
 O       0.203186     2.469165     1.089267     160.22
 C      -0.039146     0.029195     0.126884      59.19
 H       0.959704    -0.182044     0.267215      22.46
 C      -2.287112    -0.726507    -0.379439      38.18
 C      -3.299788    -1.772878    -0.812781      81.79
 H      -4.132596    -1.217186    -1.367688      21.59
 O      -2.777165    -2.396219    -2.103422     297.53
 H      -2.970173    -3.309917    -1.800331      22.11
 C      -4.006579    -2.795656     0.157659      95.70
 H      -3.583253    -3.679052     0.661566      22.03
 O      -4.492935    -2.070419     1.316224     367.58
 H      -3.865833    -1.946591     2.043011      29.07
 C      -5.305056    -3.345730    -0.656852      68.80
 O      -4.676052    -4.515329    -1.585213     174.72
 H      -4.617809    -5.274355    -0.931648      31.24
 H      -5.559998    -2.674814    -1.656783      25.98
 H      -6.039082    -3.644808    -0.035156      28.47
55
name = lig-etoh-frame_279
 C       2.869132     2.182458    -1.933008      50.09
 H       2.212219     2.805761    -2.535108      21.56
 C       3.734929     1.260558     0.204455      56.38
 H       3.657092     1.118300     1.235320      22.47
 C       4.271396     0.165991    -0.571504      -8.72
 O       4.992001    -1.021314     0.075873     149.02
 C       5.231713    -0.822583     1.572766     106.65
 H       4.342204    -0.973647     2.339434      25.13
 H       5.905943     0.080973     1.791457      25.98
 H       5.837705    -1.705526     1.766997      27.16
 C       4.250855     0.120570    -1.977596       5.15
 O       4.769730    -1.200498    -2.662529     147.52
 H       5.156175    -1.707406    -1.805525      20.81
 C       3.348480     0.982451    -2.610575      61.36
 H       3.450915     1.108725    -3.739298      25.50
 C       2.903748     2.159802    -0.525485      28.63
 C       2.365294     3.355781     0.231237     110.29
 H       2.842740     4.280615    -0.333295      23.02
 O       2.716503     3.321726     1.591299     290.96
 H       3.717809     3.451299     1.862629      26.94
 C       0.820666     3.377153     0.086623      70.14
 H       0.579335     3.055361    -0.885106      23.23
 C       0.314615     4.857386     0.257720     118.81
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 O       0.792082     5.683017    -0.702547     256.44
 H       0.259024     5.315273    -1.605284      23.84
 H       0.814325     5.170169     1.182861      25.90
 H      -0.740685     4.876330     0.397520      25.97
 C      -1.003238    -0.906303    -0.288198      64.51
 H      -0.669684    -1.800800    -0.857329      20.89
 C      -2.849651     0.478234     0.261474      62.15
 H      -3.953113     0.503234     0.596752      21.30
 C      -1.978244     1.546617     0.642765       3.41
 O      -2.436455     2.927540     0.803609     171.34
 C      -3.823556     3.299999     0.912669     102.16
 H      -4.147145     4.325398     0.317241      24.50
 H      -4.477995     2.395344     0.263280      22.95
 H      -4.159683     3.337855     2.054547      25.05
 C      -0.589689     1.263955     0.541771     -12.97
 O       0.212846     2.472754     1.096916     133.33
 C      -0.013203    -0.039633     0.087141      40.65
 H       1.110549     0.107755     0.444213      19.44
 C      -2.320202    -0.681017    -0.268003      40.34
 C      -3.263456    -1.761773    -0.829624      80.10
 H      -4.076441    -1.161085    -1.173979      23.93
 O      -2.828030    -2.477812    -2.113438     276.00
 H      -3.122700    -3.425711    -2.206793      20.13
 C      -4.064815    -2.759880     0.167895      87.44
 H      -3.561759    -3.689220     0.531619      21.82
 O      -4.506907    -2.038330     1.331213     318.46
 H      -3.751690    -1.606532     2.019198      22.84
 C      -5.241208    -3.220011    -0.651088      77.84
 O      -4.687205    -4.584060    -1.599986      67.42
 H      -4.484793    -5.199512    -0.786412      28.04
 H      -5.682217    -2.767803    -1.434120      29.25
 H      -6.204293    -3.705684    -0.100445      25.94
55
name = lig-etoh-frame_280
 C       2.852799     2.156958    -1.861332      35.04
 H       2.215430     2.794227    -2.485265      21.14
 C       3.768243     1.172582     0.180820      64.60
 H       3.725375     1.351198     1.314876      20.35
 C       4.289972     0.197248    -0.525797       8.74
 O       4.989436    -1.068096     0.112290     172.31
 C       5.189142    -0.792727     1.532594     127.45
 H       4.490461    -0.930409     2.314219      28.17
 H       5.874681    -0.013833     1.740074      28.83
 H       5.936227    -1.629087     1.668405      27.27
 C       4.245635     0.133964    -1.971723       6.91
 O       4.711564    -1.198999    -2.635721     188.62
 H       4.945553    -1.747230    -1.922748      23.93
 C       3.398124     1.062554    -2.621506      68.77
 H       3.181857     1.184005    -3.703166      26.29
 C       2.898372     2.234878    -0.494458      39.93
 C       2.324123     3.434348     0.258098     128.91
 H       2.986090     4.182926    -0.320116      23.00
 O       2.730225     3.340392     1.602027     341.47
 H       3.606950     3.540917     1.745166      31.44
 C       0.825095     3.357647     0.070023      63.76
 H       0.743954     2.867253    -0.976514      19.20
 C       0.309016     4.811351     0.334522     102.14
 O       0.724770     5.721657    -0.706720     242.62
 H       0.419193     5.565001    -1.627837      27.48
 H       1.000046     5.159719     1.181649      24.15
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 H      -0.851903     4.676300     0.280600      22.47
 C      -0.984283    -0.924773    -0.373232      35.84
 H      -0.739294    -1.931825    -0.689659      24.86
 C      -2.897349     0.555203     0.246813      81.43
 H      -3.818861     0.670857     0.707542      26.70
 C      -2.035094     1.607526     0.629738       1.05
 O      -2.352755     2.980085     0.772687     175.39
 C      -3.837455     3.256359     0.921663     136.97
 H      -4.003193     4.062467     0.333535      29.62
 H      -4.404134     2.463483     0.592208      28.96
 H      -4.090955     3.377958     1.901704      29.95
 C      -0.624600     1.290970     0.588817      -7.25
 O       0.214756     2.436182     1.079671     144.75
 C       0.006090     0.041033     0.127508      32.17
 H       1.090041    -0.066957     0.213742      21.70
 C      -2.401702    -0.678788    -0.161499      27.47
 C      -3.267353    -1.771162    -0.872464      65.58
 H      -4.158602    -1.055744    -1.036841      22.79
 O      -2.864590    -2.540836    -2.088655     253.65
 H      -3.366734    -3.369568    -2.510593      17.76
 C      -4.084983    -2.704149     0.183018      86.81
 H      -3.383677    -3.564443     0.278646      22.96
 O      -4.532839    -1.985560     1.359204     341.26
 H      -3.703441    -1.703059     1.660849      30.03
 C      -5.208722    -3.208861    -0.666826      64.88
 O      -4.713153    -4.617864    -1.564695      94.44
 H      -4.313646    -5.106808    -0.874283      29.71
 H      -5.770859    -2.436205    -1.432854      25.81
 H      -5.968034    -3.643372    -0.088860      27.20
55
name = lig-etoh-frame_281
 C       2.820819     2.104526    -1.831627      65.51
 H       2.261092     2.912591    -2.359099      25.24
 C       3.706888     1.186639     0.192706      59.53
 H       3.960757     1.399685     1.245419      23.19
 C       4.368115     0.115986    -0.514973      13.68
 O       4.942639    -1.043071     0.140292     216.96
 C       5.233204    -0.827666     1.481868     110.00
 H       4.243695    -0.802548     2.199091      24.56
 H       5.742850     0.231384     1.613960      25.66
 H       5.957521    -1.617461     1.781994      26.73
 C       4.223797     0.064542    -1.978790      10.82
 O       4.630774    -1.128058    -2.598495     198.18
 H       4.827853    -1.832753    -1.908110      24.12
 C       3.469724     1.155609    -2.632766      49.99
 H       3.069029     1.012785    -3.644099      20.67
 C       2.968242     2.245443    -0.441494      25.21
 C       2.349844     3.444004     0.259903     103.41
 H       2.763243     4.424474    -0.220160      22.10
 O       2.722980     3.369325     1.647584     269.42
 H       3.734068     3.844316     1.494462      22.27
 C       0.824434     3.345968     0.055058      65.31
 H       0.630534     2.970632    -0.918345      21.33
 C       0.289513     4.735256     0.366105      94.68
 O       0.671482     5.793534    -0.697572     236.01
 H       0.570730     5.524698    -1.726852      23.89
 H       0.721678     5.178325     1.346880      23.58
 H      -0.792986     4.694167     0.510885      24.27
 C      -0.946711    -0.911542    -0.415109      18.22
 H      -0.704299    -2.036936    -0.539171      22.68
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 C      -2.950157     0.648849     0.275133      49.91
 H      -4.070364     0.731938     0.581704      21.96
 C      -2.037647     1.662721     0.586723       8.02
 O      -2.297079     3.008038     0.753919     161.04
 C      -3.803988     3.200859     0.929831     101.98
 H      -3.932948     4.153004     0.212181      24.82
 H      -4.542216     2.250510     0.665953      22.21
 H      -4.019899     3.555839     2.083077      24.66
 C      -0.610305     1.359832     0.635390      19.43
 O       0.215886     2.375991     1.048538     167.21
 C      -0.059315     0.148822     0.168385      30.62
 H       1.028270    -0.213677    -0.041019      20.72
 C      -2.406532    -0.736941    -0.133076      -1.83
 C      -3.370610    -1.758108    -0.884725      75.84
 H      -4.140796    -1.119819    -1.280221      24.61
 O      -2.875792    -2.568287    -2.050396     250.09
 H      -3.637154    -3.088153    -2.289098      23.79
 C      -4.056300    -2.650001     0.143647      91.72
 H      -3.278027    -3.415773     0.369105      24.10
 O      -4.552398    -1.949492     1.360619     288.52
 H      -3.591251    -1.727698     1.675506      25.61
 C      -5.211581    -3.265592    -0.722241      75.57
 O      -4.760231    -4.592903    -1.509863     166.49
 H      -4.075227    -5.045938    -0.898453      28.23
 H      -5.505609    -2.413016    -1.254224      27.94
 H      -5.961074    -3.673601     0.087567      25.33
55
name = lig-etoh-frame_282
 C       2.795910     2.084767    -1.824345      76.23
 H       2.305579     2.926827    -2.270130      25.92
 C       3.670080     1.215735     0.218905      62.12
 H       4.061006     1.317133     1.220665      24.12
 C       4.412893     0.047349    -0.534588      17.95
 O       4.880600    -0.999107     0.128274     250.22
 C       5.284903    -0.830907     1.483231     131.04
 H       4.353361    -0.746520     1.920455      27.50
 H       5.557287     0.168916     1.531079      28.31
 H       5.904705    -1.606785     1.931389      27.58
 C       4.179390    -0.000753    -1.937675      14.40
 O       4.546571    -1.045486    -2.578598     192.66
 H       4.752373    -1.827604    -1.905380      23.29
 C       3.547825     1.183746    -2.624342      45.16
 H       3.144566     0.814497    -3.634749      21.88
 C       3.070832     2.218310    -0.417670      37.42
 C       2.400398     3.404215     0.247873      96.83
 H       2.302931     4.522557    -0.052547      19.69
 O       2.747916     3.434318     1.684939     306.47
 H       3.541747     3.985936     1.676638      27.45
 C       0.821039     3.342253     0.071353      52.55
 H       0.416500     3.123251    -0.987116      19.17
 C       0.251642     4.710923     0.370100      99.58
 O       0.614425     5.861637    -0.663976     204.41
 H       0.733990     5.253968    -1.519362      25.16
 H       0.508472     5.094458     1.360469      24.48
 H      -0.816252     4.715267     0.608327      24.24
 C      -0.975384    -0.862610    -0.367923      55.04
 H      -0.522636    -1.798923    -0.548153      25.22
 C      -2.988839     0.660736     0.306494      45.92
 H      -4.038514     0.685276     0.202600      20.41
 C      -1.997942     1.691756     0.536884      -0.17
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 O      -2.297559     3.014854     0.750038     195.32
 C      -3.756301     3.205553     0.947824     134.64
 H      -4.040750     3.968730     0.277456      28.42
 H      -4.438439     2.357313     0.756390      25.93
 H      -3.847764     3.572883     1.860325      29.60
 C      -0.588871     1.415909     0.643194      28.45
 O       0.244949     2.341091     1.027844     191.01
 C      -0.163108     0.189941     0.163992      41.37
 H       0.941163     0.027150    -0.111700      21.73
 C      -2.364063    -0.757349    -0.177856       6.67
 C      -3.469063    -1.687714    -0.878586      69.08
 H      -4.174307    -1.090339    -1.570962      21.38
 O      -2.875268    -2.565603    -1.982478     237.08
 H      -3.777230    -2.955430    -2.135360      23.46
 C      -4.026474    -2.633130     0.084251      92.12
 H      -3.313480    -3.306623     0.599583      22.88
 O      -4.539883    -1.926904     1.325588     273.70
 H      -3.774838    -1.700672     2.062599      23.35
 C      -5.202535    -3.401745    -0.702051      82.01
 O      -4.819858    -4.527213    -1.437324     262.22
 H      -3.920281    -4.815206    -1.030300      28.59
 H      -5.551795    -2.558392    -1.448861      25.96
 H      -6.044601    -3.552551     0.034890      26.07
55
name = lig-etoh-frame_283
 C       2.826421     2.082803    -1.835144      65.93
 H       2.247492     2.907347    -2.344356      24.26
 C       3.740080     1.153377     0.244415      54.94
 H       3.973543     1.297384     1.389872      21.95
 C       4.358482     0.106871    -0.532877      29.89
 O       4.851698    -1.014767     0.094011     224.66
 C       5.302788    -0.803934     1.487087      98.29
 H       4.248570    -0.801786     2.117361      23.78
 H       5.823459     0.244986     1.630068      25.33
 H       5.940843    -1.655310     1.931581      25.57
 C       4.108290     0.042638    -1.842717      27.21
 O       4.484313    -1.037176    -2.609293     239.72
 H       4.735923    -1.698181    -2.028286      28.01
 C       3.588556     1.126563    -2.588198      46.45
 H       3.389035     0.926288    -3.607888      22.65
 C       3.127779     2.234241    -0.456435      30.09
 C       2.401553     3.367563     0.265726      98.13
 H       2.519437     4.388309    -0.170413      23.12
 O       2.752897     3.504895     1.706482     304.63
 H       3.599724     4.086481     1.913486      24.97
 C       0.806182     3.328125     0.093135      66.58
 H       0.458154     3.143039    -0.923540      22.02
 C       0.196488     4.759849     0.386149      86.34
 O       0.561026     5.873667    -0.590419     244.92
 H       0.693307     5.424482    -1.403704      31.85
 H       0.653386     5.062467     1.466137      22.48
 H      -0.989204     4.593973     0.311388      22.45
 C      -1.035258    -0.808657    -0.272234      67.17
 H      -0.334912    -1.600493    -0.768732      21.10
 C      -2.926760     0.585074     0.291271      68.07
 H      -3.983794     0.736137    -0.099032      19.73
 C      -1.993812     1.684677     0.499954      11.59
 O      -2.334670     3.011163     0.750006     207.86
 C      -3.690837     3.244962     0.948383     113.45
 H      -4.180375     3.999809     0.168308      25.83
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 H      -4.341801     2.297518     0.855104      25.20
 H      -3.794184     3.693601     2.101773      24.78
 C      -0.623128     1.417611     0.600192      20.92
 O       0.319740     2.360192     1.029898     201.36
 C      -0.228889     0.205429     0.126518      45.17
 H       0.867858     0.293224     0.036640      21.01
 C      -2.388230    -0.689998    -0.253993      32.03
 C      -3.473982    -1.574300    -0.893757      80.78
 H      -4.217620    -0.990283    -1.417464      24.95
 O      -2.878603    -2.544185    -1.894804     250.66
 H      -3.622455    -3.085955    -2.395222      23.91
 C      -4.040251    -2.636832     0.090755      83.83
 H      -3.252078    -3.305929     0.507392      24.20
 O      -4.536694    -1.903009     1.288210     322.23
 H      -4.030092    -1.869973     2.024888      31.68
 C      -5.215999    -3.452043    -0.639803     100.78
 O      -4.852238    -4.493021    -1.372082     287.11
 H      -3.962221    -4.675069    -1.219259      33.26
 H      -5.739199    -2.981735    -1.495315      25.56
 H      -6.145497    -3.596502     0.017425      26.70
55
name = lig-etoh-frame_284
 C       2.908116     2.105721    -1.869207      76.17
 H       2.274274     2.751551    -2.433512      23.65
 C       3.830886     1.134073     0.280410      84.01
 H       3.793884     1.234534     1.281001      26.23
 C       4.269046     0.183562    -0.438416      27.89
 O       4.860190    -1.054416     0.078028     191.67
 C       5.281876    -0.765758     1.511317     124.56
 H       4.581317    -0.780079     2.249737      28.83
 H       6.002588    -0.014565     1.672646      29.23
 H       5.907250    -1.619500     1.665827      28.45
 C       4.054389     0.093132    -1.832038      29.61
 O       4.429256    -1.047954    -2.656489     186.06
 H       4.850756    -1.772507    -2.064916      24.72
 C       3.561194     1.071683    -2.533140      48.46
 H       3.675729     1.136855    -3.694375      20.24
 C       3.140241     2.234490    -0.482829      44.62
 C       2.393217     3.374300     0.294887     103.10
 H       3.055606     4.100686    -0.394240      20.60
 O       2.730700     3.568770     1.714275     267.51
 H       3.736690     4.007720     1.799370      23.58
 C       0.815640     3.349304     0.120797      66.31
 H       0.639243     2.976842    -0.935045      21.07
 C       0.139729     4.816972     0.407059     112.20
 O       0.517907     5.861037    -0.481273     249.24
 H       0.514583     5.675690    -1.570545      25.58
 H       0.529673     5.083039     1.323365      26.04
 H      -0.855171     4.621599     0.233984      25.76
 C      -1.043398    -0.821051    -0.220572      60.20
 H      -0.610021    -1.482864    -0.902516      23.55
 C      -2.839541     0.516474     0.217578      76.82
 H      -3.805803     0.882048    -0.120778      22.59
 C      -2.033814     1.662841     0.490012      18.37
 O      -2.363963     2.993557     0.740347     221.51
 C      -3.689432     3.323519     0.980952     131.21
 H      -4.124594     3.937546     0.197708      28.00
 H      -4.212724     2.271826     1.109181      24.96
 H      -3.811734     3.718148     1.901410      29.73
 C      -0.679012     1.442555     0.555440      14.64
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 O       0.384114     2.376486     1.043300     150.71
 C      -0.221529     0.247008     0.102844      33.59
 H       0.983385     0.215894     0.197737      20.75
 C      -2.469247    -0.584100    -0.330394      35.90
 C      -3.441504    -1.521965    -0.909981      76.18
 H      -4.333582    -0.847949    -1.195233      24.56
 O      -2.868285    -2.510213    -1.831177     302.74
 H      -3.305076    -2.979890    -2.490804      29.08
 C      -4.086523    -2.613586     0.141085      71.73
 H      -3.223038    -3.329082     0.199490      25.00
 O      -4.570148    -1.882969     1.227817     280.19
 H      -3.907983    -2.164964     2.068482      23.98
 C      -5.287330    -3.392513    -0.544145      82.70
 O      -4.847295    -4.551695    -1.344526     229.01
 H      -3.850609    -4.731221    -1.306207      30.25
 H      -5.929528    -2.791420    -1.305973      25.58
 H      -6.040804    -3.842708     0.243967      25.88
55
name = lig-etoh-frame_285
 C       3.003721     2.157913    -1.873142      61.82
 H       2.332186     2.788431    -2.514572      22.64
 C       3.842602     1.277031     0.320825      58.85
 H       3.668421     1.187925     1.525202      20.02
 C       4.229301     0.093625    -0.397811      16.72
 O       4.868370    -1.048151     0.100112     185.18
 C       5.304937    -0.789677     1.500865     102.29
 H       4.563965    -0.682129     2.473144      24.26
 H       6.126636     0.032118     1.546867      25.83
 H       5.892414    -1.797771     1.499998      25.06
 C       4.065569     0.030999    -1.848120      16.58
 O       4.380208    -1.056768    -2.675087     181.16
 H       4.975453    -1.739913    -2.160906      24.06
 C       3.495637     1.088028    -2.565691      64.86
 H       3.787164     1.174767    -3.549525      26.29
 C       3.114542     2.187793    -0.457955      47.89
 C       2.439299     3.403082     0.288427     115.23
 H       3.001114     4.106059    -0.257476      26.60
 O       2.718048     3.627458     1.698142     300.37
 H       3.653151     3.826790     1.586783      30.19
 C       0.866496     3.417437     0.124130      69.22
 H       0.770636     2.943480    -0.877888      23.73
 C       0.117459     4.816338     0.378077      96.86
 O       0.501960     5.873986    -0.408432     263.05
 H       0.186942     5.725727    -1.304467      30.04
 H       0.291209     5.223892     1.552652      23.77
 H      -1.117571     4.637236     0.409490      22.72
 C      -1.055808    -0.843469    -0.231338      37.37
 H      -0.824434    -1.741141    -0.927410      21.14
 C      -2.846694     0.624367     0.147209      68.59
 H      -3.892145     0.939356     0.030745      21.81
 C      -2.059929     1.660193     0.511250      31.67
 O      -2.374230     2.970075     0.724273     218.02
 C      -3.734410     3.353180     1.018703     115.90
 H      -4.142483     3.968670     0.121658      26.21
 H      -4.323174     2.447720     1.230430      26.10
 H      -3.817715     4.042366     2.050178      25.26
 C      -0.674970     1.508743     0.535908      11.03
 O       0.399110     2.364929     1.061561     146.45
 C      -0.145402     0.256617     0.105303      35.60
 H       0.842160    -0.021709     0.168439      23.08
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 C      -2.444759    -0.589286    -0.418051      28.91
 C      -3.471077    -1.536334    -0.919197      91.08
 H      -4.338762    -0.937860    -1.222016      26.26
 O      -2.810752    -2.450553    -1.789391     285.09
 H      -3.358167    -2.769771    -2.587634      26.40
 C      -4.138048    -2.565915     0.136019      83.15
 H      -3.325333    -3.315091     0.210162      25.80
 O      -4.586904    -1.878246     1.220603     321.10
 H      -3.968440    -2.221945     1.923682      27.22
 C      -5.353262    -3.347490    -0.454639      77.65
 O      -4.841747    -4.622292    -1.332629     188.23
 H      -3.826516    -4.675255    -1.204095      28.77
 H      -5.993416    -2.526969    -0.864444      26.98
 H      -5.808016    -3.877201     0.417544      27.24
55
name = lig-etoh-frame_286
 C       3.067863     2.230845    -1.858570      51.96
 H       2.548391     3.037904    -2.372940      23.12
 C       3.822101     1.373133     0.366778      60.08
 H       3.725727     1.334207     1.353996      22.34
 C       4.196035    -0.012434    -0.421892      10.70
 O       4.862206    -1.010903     0.158759     219.30
 C       5.383322    -0.866739     1.492842     129.51
 H       4.630501    -0.647538     2.142871      28.54
 H       5.976228     0.009440     1.392557      28.14
 H       5.817862    -1.785999     1.735258      28.41
 C       4.083570    -0.048096    -1.848638      17.80
 O       4.351673    -1.079906    -2.676947     229.39
 H       4.968311    -1.630218    -2.290821      28.36
 C       3.467293     1.096624    -2.594139      35.32
 H       3.674098     1.106718    -3.742163      23.25
 C       3.055048     2.178308    -0.400725      43.99
 C       2.468750     3.436384     0.269923      97.21
 H       2.698954     4.570840    -0.187545      22.18
 O       2.709431     3.672511     1.662594     231.24
 H       3.857623     3.732114     1.669236      24.68
 C       0.931863     3.484420     0.122051      57.59
 H       0.679598     3.160232    -0.898506      22.39
 C       0.062338     4.777258     0.425265     122.92
 O       0.494858     5.916451    -0.363553     261.67
 H       0.008321     5.718986    -1.195481      29.25
 H       0.138771     5.069949     1.370686      28.46
 H      -0.914569     4.628676     0.420032      27.26
 C      -1.063705    -0.859271    -0.314261      55.04
 H      -0.739297    -1.885871    -0.527044      23.87
 C      -2.942854     0.761067     0.050849      54.56
 H      -4.058121     0.852661     0.227913      27.05
 C      -2.030077     1.700006     0.545398      10.05
 O      -2.409177     2.974392     0.726097     194.36
 C      -3.789227     3.401761     1.077700     120.35
 H      -4.163517     3.890157     0.136606      27.02
 H      -4.658508     2.604756     1.371886      25.92
 H      -3.664933     4.177900     1.761416      27.91
 C      -0.568724     1.522701     0.523337      19.41
 O       0.375915     2.357738     1.070739     172.64
 C      -0.128912     0.221473     0.113147      25.87
 H       1.039889    -0.213131     0.128618      20.90
 C      -2.388662    -0.593172    -0.448615      21.50
 C      -3.524570    -1.582907    -0.904979      86.70
 H      -4.335982    -1.045567    -1.552949      23.65
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 O      -2.740031    -2.400945    -1.803680     294.63
 H      -3.472899    -2.489576    -2.509235      24.95
 C      -4.163299    -2.531988     0.062947     107.00
 H      -3.423026    -3.257197     0.521786      22.65
 O      -4.601363    -1.868195     1.265438     320.53
 H      -4.049064    -2.033150     1.999010      30.75
 C      -5.367937    -3.339415    -0.372619      74.34
 O      -4.858663    -4.647034    -1.314533     191.27
 H      -3.975040    -4.551339    -1.048189      30.22
 H      -6.151286    -2.626445    -0.700783      26.79
 H      -5.678763    -3.888254     0.654755      25.68
55
name = lig-etoh-frame_287
 C       3.108263     2.273283    -1.840366      35.45
 H       2.836691     3.292505    -2.218884      19.72
 C       3.806681     1.319633     0.331587      54.03
 H       3.851488     1.501951     1.544683      16.93
 C       4.151130    -0.005057    -0.437906      16.08
 O       4.860892    -1.020389     0.212676     225.76
 C       5.453763    -0.924419     1.462276     112.28
 H       4.452770    -0.591929     2.084048      23.89
 H       6.113151     0.009957     1.474585      26.71
 H       5.926646    -1.847053     2.032059      25.07
 C       4.052206    -0.051221    -1.852210      12.73
 O       4.334251    -1.127092    -2.688736     193.24
 H       5.086605    -1.737698    -2.304963      24.23
 C       3.488653     1.096929    -2.589229      40.20
 H       3.319598     1.000132    -3.649663      23.91
 C       3.003110     2.264832    -0.374481      49.01
 C       2.448061     3.548381     0.244480     111.25
 H       2.533922     4.451574    -0.246151      24.95
 O       2.747375     3.694603     1.633884     347.11
 H       3.610264     3.861910     1.835849      34.10
 C       0.948662     3.520760     0.121978      50.64
 H       0.572699     3.394523    -0.946581      20.16
 C       0.067206     4.734057     0.485342      76.51
 O       0.478145     5.955587    -0.329835     151.43
 H       0.014881     5.836371    -1.319265      26.12
 H       0.241345     4.996247     1.701712      22.72
 H      -1.112538     4.414462     0.132957      19.32
 C      -1.028063    -0.851765    -0.390842      57.68
 H      -0.560626    -1.854137    -0.184426      23.37
 C      -3.005230     0.810338    -0.054865      43.34
 H      -4.021615     0.812044     0.259193      24.13
 C      -1.984867     1.735694     0.541396     -20.27
 O      -2.466770     3.017684     0.764527     149.86
 C      -3.849363     3.437248     1.095687     116.80
 H      -4.261219     3.840207     0.120984      26.36
 H      -4.577806     2.799903     1.516041      27.80
 H      -3.629784     4.301505     1.805999      25.66
 C      -0.463490     1.455699     0.501969      10.37
 O       0.354517     2.380522     1.066758     152.43
 C      -0.118401     0.136156     0.114023      38.46
 H       0.849595    -0.013784     0.151649      23.73
 C      -2.445575    -0.513145    -0.413686      -4.17
 C      -3.529489    -1.591101    -0.908097      95.07
 H      -4.166895    -1.146040    -1.656597      23.95
 O      -2.689357    -2.371473    -1.866927     294.81
 H      -3.303472    -2.550224    -2.539216      29.06
 C      -4.160935    -2.526051     0.057889      95.70
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 H      -3.423047    -3.175423     0.537937      22.75
 O      -4.640834    -1.833964     1.315785     237.68
 H      -3.895214    -1.776741     2.149383      23.57
 C      -5.361134    -3.395507    -0.286406      93.03
 O      -4.909451    -4.611407    -1.276880     207.37
 H      -3.946401    -4.568141    -0.927797      28.38
 H      -6.338979    -3.037222    -0.785642      25.66
 H      -5.676671    -3.815267     0.606555      28.12
55
name = lig-etoh-frame_288
 C       3.130349     2.293715    -1.803798      63.12
 H       3.096402     3.274676    -2.311553      22.41
 C       3.748117     1.207872     0.280977      70.86
 H       4.078627     1.449746     1.235385      21.65
 C       4.129252     0.082339    -0.394364      10.99
 O       4.864025    -1.077139     0.209140     212.80
 C       5.469853    -0.911065     1.501834     134.73
 H       4.753166    -0.662836     2.192654      28.39
 H       6.292936    -0.209398     1.667643      29.11
 H       5.911873    -1.792683     1.847366      29.20
 C       3.988538    -0.017545    -1.876806      19.27
 O       4.330244    -1.187807    -2.692873     183.00
 H       5.049031    -1.768850    -2.250337      24.55
 C       3.508553     1.110815    -2.527122      59.99
 H       3.101718     0.958101    -3.560896      21.66
 C       3.026830     2.362377    -0.395002      62.82
 C       2.405692     3.643845     0.244450      87.12
 H       2.787396     4.514929    -0.584438      23.55
 O       2.742603     3.702066     1.619555     246.92
 H       3.815280     4.164286     1.760679      21.98
 C       0.887318     3.532901     0.120962      66.93
 H       0.698263     3.338162    -0.906544      21.95
 C       0.068262     4.718716     0.552046     117.55
 O       0.446847     5.977874    -0.298277     230.98
 H       0.274370     5.888149    -1.187239      33.66
 H       0.155352     4.916996     1.498796      28.68
 H      -0.784309     4.427658     0.231059      26.92
 C      -1.009834    -0.815672    -0.421761      49.53
 H      -0.657504    -1.853496    -0.183502      23.42
 C      -2.955291     0.812897    -0.121815      52.75
 H      -4.069914     0.917857     0.148319      23.46
 C      -1.971777     1.744768     0.475456     -23.03
 O      -2.508697     3.067004     0.829187     138.65
 C      -3.879279     3.491379     1.082849     104.66
 H      -4.455870     3.781344     0.122959      25.45
 H      -4.448260     2.654078     1.804157      24.23
 H      -3.810716     4.323378     1.912165      24.79
 C      -0.476264     1.388421     0.480520       9.09
 O       0.359224     2.421847     1.046420     153.10
 C      -0.132334     0.086207     0.107176      34.10
 H       1.112180    -0.016830     0.218252      19.17
 C      -2.539841    -0.437665    -0.370065       3.61
 C      -3.461060    -1.561503    -0.953923      78.38
 H      -4.283583    -1.011714    -1.529329      23.51
 O      -2.639425    -2.360858    -1.940774     233.43
 H      -3.147062    -2.836026    -2.694657      24.02
 C      -4.166511    -2.521311     0.143408      70.60
 H      -3.280254    -3.231114     0.315466      23.50
 O      -4.670010    -1.783449     1.372516     275.86
 H      -3.862667    -1.602632     1.817693      28.71
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 C      -5.364243    -3.506082    -0.268179      89.27
 O      -4.955513    -4.526298    -1.203291     224.01
 H      -4.015942    -4.889225    -1.008696      28.69
 H      -6.198365    -3.239626    -0.842088      26.01
 H      -5.764467    -3.947331     0.843294      24.64
55
name = lig-etoh-frame_289
 C       3.154368     2.323300    -1.767560      58.75
 H       3.084242     3.118273    -2.525189      26.40
 C       3.638966     1.170331     0.225586      83.10
 H       4.224950     1.298727     1.239336      24.94
 C       4.158830     0.104446    -0.389340       9.11
 O       4.863802    -1.107542     0.179781     154.38
 C       5.487368    -0.887394     1.557637     103.33
 H       4.820228    -0.646484     2.542884      24.12
 H       6.425601    -0.264256     1.607902      26.92
 H       5.874346    -2.023593     1.563108      24.47
 C       3.942090    -0.021170    -1.877522       7.96
 O       4.318661    -1.223308    -2.671386     216.60
 H       4.881758    -1.709311    -2.121742      27.44
 C       3.501135     1.126562    -2.468257      58.67
 H       3.133632     1.055653    -3.521283      21.07
 C       3.110415     2.411036    -0.433083      41.67
 C       2.400001     3.701833     0.213892     101.55
 H       2.832575     4.402189    -0.361546      27.77
 O       2.756129     3.740687     1.616006     331.62
 H       3.604296     4.054156     1.458895      29.53
 C       0.828367     3.523477     0.125659      64.45
 H       0.731321     3.137705    -0.962290      21.10
 C       0.102476     4.751700     0.534719      90.72
 O       0.422253     5.988824    -0.226491     191.62
 H       0.445289     5.686154    -1.252023      28.13
 H       0.099130     5.051727     1.750844      22.86
 H      -1.149233     4.471427     0.358345      19.93
 C      -1.078950    -0.787060    -0.403199      27.71
 H      -0.927013    -1.870380    -0.541638      23.64
 C      -2.895577     0.856934    -0.116983      56.50
 H      -3.913441     1.159588    -0.185532      26.90
 C      -1.984755     1.759626     0.380631       0.60
 O      -2.508328     3.103750     0.893210     150.45
 C      -3.916893     3.490776     1.117181     121.49
 H      -4.558339     3.704499     0.234638      27.64
 H      -4.278253     2.693366     1.646674      28.67
 H      -3.911585     4.389475     1.751209      27.03
 C      -0.590413     1.412797     0.477495       4.14
 O       0.371241     2.443273     1.007519     152.46
 C      -0.069514     0.094257     0.107304      41.21
 H       0.868568    -0.223092     0.228743      22.42
 C      -2.533187    -0.476909    -0.384875      23.87
 C      -3.423024    -1.515956    -1.022549      69.69
 H      -4.335160    -0.976288    -1.323213      23.55
 O      -2.594162    -2.346624    -2.013009     204.24
 H      -3.142194    -3.062478    -2.515723      22.24
 C      -4.175266    -2.526172     0.236492      62.37
 H      -3.322628    -3.210240     0.313099      23.87
 O      -4.666590    -1.748975     1.383496     284.86
 H      -3.782652    -1.396587     1.729949      25.59
 C      -5.353566    -3.621298    -0.215153     101.92
 O      -4.973657    -4.466053    -1.142639     304.50
 H      -4.302970    -5.078784    -0.978519      32.41
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 H      -6.196861    -2.964382    -0.784500      25.15
 H      -5.688127    -4.003538     0.661759      28.71
55
name = lig-etoh-frame_290
 C       3.190662     2.350230    -1.813772      48.61
 H       2.783656     3.097134    -2.549483      23.48
 C       3.551664     1.219979     0.239966      64.12
 H       3.932605     1.189500     1.280163      24.95
 C       4.207684     0.025403    -0.474286       5.89
 O       4.851867    -1.063977     0.167226     175.43
 C       5.519411    -0.927380     1.606933     111.65
 H       4.922391    -0.681701     2.416606      27.61
 H       6.345204    -0.252769     1.384280      27.62
 H       5.761357    -1.930741     1.556377      27.62
 C       3.934741    -0.077767    -1.843767      13.24
 O       4.287468    -1.212752    -2.625500     193.55
 H       4.776254    -1.801054    -1.879129      21.58
 C       3.469461     1.134732    -2.448018      48.09
 H       3.357727     1.186941    -3.522393      23.33
 C       3.192172     2.432009    -0.421771      35.49
 C       2.396586     3.647134     0.211173      80.84
 H       2.788947     4.771875    -0.261230      22.19
 O       2.734132     3.786867     1.595789     245.81
 H       3.877854     3.968987     1.590841      21.89
 C       0.808364     3.487439     0.099075      76.84
 H       0.541368     3.195691    -0.879726      24.70
 C       0.038954     4.824336     0.525039     127.53
 O       0.405659     5.983376    -0.173377     234.12
 H       0.622367     5.513102    -1.076147      30.30
 H       0.262782     5.008324     1.507287      27.66
 H      -0.931407     4.722987     0.559557      28.01
 C      -1.174252    -0.778894    -0.340692      36.79
 H      -1.009322    -1.710517    -1.007563      21.09
 C      -2.875451     0.879358    -0.108107      59.79
 H      -3.819829     1.373150    -0.545019      20.92
 C      -2.009299     1.836448     0.320013      16.85
 O      -2.469792     3.124688     0.937091     138.54
 C      -3.927012     3.456341     1.148534      92.89
 H      -4.584563     3.560560     0.157268      25.39
 H      -4.458666     2.493362     1.721665      24.16
 H      -3.904956     4.578753     1.604536      24.49
 C      -0.656853     1.483768     0.485342       1.47
 O       0.366307     2.429281     0.967227     167.06
 C      -0.102376     0.140974     0.099763      27.05
 H       0.992915    -0.380963     0.269192      19.24
 C      -2.451311    -0.530463    -0.445715      40.02
 C      -3.428720    -1.499815    -1.054703      66.49
 H      -4.321589    -1.014759    -1.515950      25.11
 O      -2.583064    -2.324777    -2.067025     233.22
 H      -3.177856    -3.043893    -2.151166      25.78
 C      -4.179676    -2.552075     0.291338      63.25
 H      -3.310400    -3.169312     0.708532      22.55
 O      -4.619534    -1.735574     1.360061     253.14
 H      -3.851154    -1.126767     1.846295      24.10
 C      -5.350596    -3.576270    -0.136090      92.00
 O      -4.969628    -4.464620    -1.162563     245.45
 H      -4.499144    -5.276421    -0.683960      26.85
 H      -6.060013    -2.880453    -0.386212      28.62
 H      -5.799150    -4.242648     0.853033      25.14
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name = lig-etoh-frame_291
 C       3.208515     2.366868    -1.897437      52.15
 H       2.585473     3.139520    -2.335815      22.78
 C       3.538613     1.234220     0.256713      34.71
 H       3.461054     1.237941     1.413551      22.19
 C       4.213306    -0.006579    -0.508955      19.06
 O       4.828972    -0.996830     0.173445     202.01
 C       5.543699    -0.970298     1.564384      90.94
 H       4.775548    -0.600721     2.393552      24.48
 H       6.318972    -0.210989     1.359685      26.29
 H       5.898414    -2.070707     1.813718      24.92
 C       3.938758    -0.120513    -1.832167      27.31
 O       4.260431    -1.193196    -2.548008     225.28
 H       4.586831    -1.930729    -1.972939      24.92
 C       3.445594     1.123422    -2.465769      62.70
 H       3.626014     1.173830    -3.607491      24.90
 C       3.233589     2.449228    -0.400916      26.06
 C       2.421086     3.604234     0.210774      98.55
 H       2.453751     4.496207    -0.238538      27.15
 O       2.736822     3.833840     1.583603     340.68
 H       3.608073     3.853943     1.843245      32.08
 C       0.789516     3.475666     0.073141      57.16
 H       0.385112     3.325983    -1.005290      23.42
 C       0.012091     4.864406     0.546442      95.36
 O       0.418679     5.980504    -0.167803     222.20
 H       0.676395     5.727056    -1.009394      33.63
 H       0.549929     4.975155     1.660572      23.46
 H      -1.246915     4.763158     0.564846      22.92
 C      -1.138111    -0.805029    -0.298131      53.28
 H      -0.766832    -1.493258    -0.985220      23.29
 C      -2.908719     0.859328    -0.149252      58.35
 H      -3.737972     1.246873    -0.700242      22.37
 C      -2.037411     1.953180     0.323727      -0.13
 O      -2.430265     3.129977     0.958909     153.16
 C      -3.932456     3.386768     1.156310     120.83
 H      -4.385791     3.406106     0.168429      27.65
 H      -4.448938     2.770158     1.784559      29.47
 H      -3.894167     4.335864     1.562149      29.02
 C      -0.609199     1.532218     0.489700       8.00
 O       0.340827     2.389630     0.939854     183.66
 C      -0.218874     0.197776     0.101478      36.82
 H       0.815048    -0.053661     0.234545      22.06
 C      -2.483283    -0.470790    -0.504661      23.68
 C      -3.440583    -1.523719    -1.064804      62.27
 H      -4.185330    -1.101768    -1.794810      23.72
 O      -2.622207    -2.294558    -2.089936     220.62
 H      -3.147174    -3.183960    -1.908100      22.87
 C      -4.120124    -2.593851     0.344757      78.97
 H      -3.317893    -3.063927     0.916940      23.52
 O      -4.579620    -1.703169     1.334269     312.71
 H      -3.972018    -1.230303     1.776879      31.12
 C      -5.334686    -3.495257     0.012252      91.45
 O      -4.949830    -4.491194    -1.198463     229.67
 H      -4.796833    -5.204682    -0.520885      28.67
 H      -6.301869    -2.818020    -0.241465      26.74
 H      -5.650642    -4.089352     0.729779      28.96
55
name = lig-etoh-frame_292
 C       3.206059     2.367713    -1.906884      56.25
 H       2.606892     3.219802    -2.349240      20.81
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 C       3.586675     1.223898     0.268343      46.82
 H       2.977155     1.187609     1.237049      20.90
 C       4.165005     0.073040    -0.421018      16.57
 O       4.822914    -0.980228     0.202864     234.37
 C       5.526264    -0.990974     1.486633     118.07
 H       4.806341    -0.586933     2.178945      26.81
 H       6.362770    -0.261657     1.550023      27.10
 H       5.966182    -1.877549     1.911760      27.39
 C       3.929038    -0.081473    -1.829142      13.80
 O       4.239162    -1.207674    -2.503214     220.55
 H       4.498640    -1.977548    -2.042435      26.26
 C       3.460935     1.095082    -2.539708      70.63
 H       3.628705     1.000611    -3.563189      27.02
 C       3.232576     2.430426    -0.433614      43.95
 C       2.423651     3.543072     0.221646      78.66
 H       2.451451     4.518580    -0.615558      24.93
 O       2.687831     3.868276     1.593645     247.36
 H       3.753109     3.847466     1.771240      24.60
 C       0.746533     3.483843     0.053827      54.11
 H       0.523800     3.355953    -0.982592      24.33
 C       0.007465     4.844599     0.622373     110.85
 O       0.452060     6.008491    -0.181763     165.09
 H       0.638366     5.908219    -1.235243      27.63
 H       0.456972     4.955571     1.579690      26.94
 H      -1.001338     4.738057     0.570916      27.25
 C      -1.071242    -0.803602    -0.282161      41.99
 H      -0.411674    -1.674179    -0.742889      20.04
 C      -2.939051     0.876400    -0.211764      55.72
 H      -3.978372     1.050924    -0.654901      21.28
 C      -2.031896     1.982739     0.357184       6.04
 O      -2.420191     3.125534     0.976433     154.01
 C      -3.885183     3.316239     1.132492      94.69
 H      -4.309813     3.254900     0.002762      23.87
 H      -4.442630     2.711331     2.048547      24.08
 H      -3.924261     4.457986     1.643414      24.51
 C      -0.615119     1.560401     0.469360      31.18
 O       0.333074     2.364267     0.927015     183.59
 C      -0.355983     0.284244     0.120950      43.02
 H       0.816410     0.222128     0.171692      21.74
 C      -2.548764    -0.387425    -0.546381      11.47
 C      -3.435790    -1.560960    -1.081010      65.16
 H      -4.248922    -1.153382    -1.685679      24.80
 O      -2.697065    -2.294222    -2.076924     253.09
 H      -2.813186    -3.282084    -1.980465      25.98
 C      -4.036573    -2.591804     0.386570      75.56
 H      -3.153784    -3.196541     0.734623      23.76
 O      -4.582927    -1.661376     1.302652     270.45
 H      -3.727516    -1.302657     1.831348      23.99
 C      -5.311445    -3.385483     0.081253      82.78
 O      -4.946348    -4.490124    -1.188247     194.74
 H      -4.900313    -5.260344    -0.663178      30.57
 H      -6.200206    -2.968191    -0.212877      28.33
 H      -5.513219    -4.185382     1.056770      24.97
55
name = lig-etoh-frame_293
 C       3.191092     2.343469    -1.879223      71.30
 H       2.903703     3.158206    -2.532071      25.36
 C       3.609373     1.234663     0.275972      70.71
 H       3.003318     1.034841     1.126484      21.15
 C       4.105534     0.172198    -0.311390      17.57
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 O       4.827326    -1.007227     0.222807     217.15
 C       5.495253    -0.940605     1.422915     117.89
 H       4.747139    -0.586044     2.240375      25.55
 H       6.376800    -0.284739     1.557776      26.38
 H       5.878793    -1.985864     1.709081      25.97
 C       3.926995     0.007539    -1.784870      23.29
 O       4.216028    -1.227918    -2.497633     137.49
 H       4.562522    -2.002308    -1.832889      21.88
 C       3.499344     1.076391    -2.595331      72.65
 H       3.416961     0.866305    -3.754672      18.23
 C       3.194839     2.366206    -0.501541      54.42
 C       2.373642     3.541074     0.175793     105.18
 H       2.727935     4.246077    -0.466298      29.82
 O       2.653507     3.883670     1.599247     287.71
 H       3.647424     4.005152     1.429783      26.99
 C       0.739446     3.507187     0.081598      63.32
 H       0.590791     3.256615    -1.020482      22.16
 C       0.083941     4.799598     0.628283      93.21
 O       0.498960     6.050566    -0.204211     170.58
 H       0.322336     5.772269    -1.155367      30.05
 H       0.358549     5.034171     1.712125      25.15
 H      -1.138335     4.673966     0.613332      22.38
 C      -1.070400    -0.778063    -0.306361      42.86
 H      -0.548821    -1.697306    -0.271655      23.19
 C      -2.980316     0.957725    -0.276915      53.98
 H      -4.082278     1.013135    -0.258266      25.11
 C      -2.025896     1.909185     0.380648      19.10
 O      -2.436798     3.122149     0.999568     205.86
 C      -3.835757     3.288722     1.131753     139.47
 H      -4.351074     3.158869     0.223696      29.00
 H      -4.170126     2.594256     1.797297      29.76
 H      -3.976402     4.244097     1.389703      29.53
 C      -0.755499     1.622058     0.438415      34.14
 O       0.354049     2.370116     0.926566     157.34
 C      -0.376311     0.329307     0.140160      35.93
 H       0.754473     0.292519     0.078411      20.63
 C      -2.523569    -0.403782    -0.581727      -7.20
 C      -3.442659    -1.592872    -1.066223      72.24
 H      -4.509131    -1.212580    -1.322180      23.66
 O      -2.753797    -2.316465    -2.065922     282.95
 H      -2.665513    -3.235291    -1.999473      25.69
 C      -3.971524    -2.542581     0.360104      80.50
 H      -3.136171    -3.268207     0.483921      23.47
 O      -4.549845    -1.602677     1.291915     297.65
 H      -3.717984    -1.471850     1.946187      24.57
 C      -5.235582    -3.398972     0.125883      86.72
 O      -4.957190    -4.447047    -1.139585     179.34
 H      -4.912465    -5.441870    -0.818976      29.15
 H      -6.199170    -2.850754    -0.259524      26.84
 H      -5.331251    -3.883035     0.967612      29.66
55
name = lig-etoh-frame_294
 C       3.190111     2.273967    -1.919284      77.89
 H       3.173123     3.157553    -2.613137      27.26
 C       3.575398     1.300094     0.317425      60.01
 H       3.276316     1.051539     1.463205      19.32
 C       4.110407     0.153199    -0.308821      12.90
 O       4.799329    -1.015511     0.196367     229.83
 C       5.465943    -0.887449     1.441731     118.86
 H       4.838763    -0.705521     2.345295      26.87
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 H       6.352516    -0.224275     1.341953      26.60
 H       5.658600    -1.979287     1.396581      25.31
 C       3.951954     0.061879    -1.745107      14.53
 O       4.192363    -1.235805    -2.463513     218.21
 H       4.634409    -1.702741    -1.743803      26.03
 C       3.535112     1.077074    -2.622765      34.94
 H       3.202633     0.927837    -3.592232      19.55
 C       3.104981     2.303856    -0.525015      46.79
 C       2.297260     3.536721     0.135565     113.41
 H       2.951371     4.467784    -0.375516      21.93
 O       2.638727     3.876954     1.557718     256.87
 H       3.569726     4.205469     1.534544      28.40
 C       0.792006     3.523103     0.105000      81.53
 H       0.452389     3.265301    -0.908385      23.24
 C       0.148512     4.782355     0.586682     101.17
 O       0.527983     6.052523    -0.218899     198.15
 H       0.122845     5.705326    -1.000327      31.74
 H       0.339942     5.097264     1.722633      24.42
 H      -0.935658     4.686213     0.571751      25.24
 C      -1.150816    -0.702840    -0.329261      47.43
 H      -0.881309    -1.784385     0.008405      21.25
 C      -2.993458     0.994361    -0.316156      56.89
 H      -4.016286     1.143487     0.065479      23.45
 C      -2.165637     1.859248     0.393847      14.19
 O      -2.440239     3.106022     1.003630     198.64
 C      -3.788997     3.255444     1.123531     104.28
 H      -4.546229     2.992827     0.167094      24.52
 H      -4.128743     2.326327     1.839182      24.70
 H      -4.126958     4.442397     1.379114      23.70
 C      -0.794029     1.656017     0.417152       6.12
 O       0.357867     2.390829     0.929028     155.30
 C      -0.315849     0.339981     0.131905      29.31
 H       0.760291     0.180619     0.151565      20.16
 C      -2.466554    -0.449146    -0.603758      -4.17
 C      -3.486807    -1.612236    -0.975868      89.81
 H      -4.474991    -1.292370    -1.185434      25.39
 O      -2.801198    -2.328198    -2.076157     234.47
 H      -2.776109    -3.339919    -1.800312      23.98
 C      -3.931695    -2.473694     0.244635     104.98
 H      -3.124111    -3.139031     0.605475      24.61
 O      -4.461005    -1.554293     1.305370     317.35
 H      -3.930407    -1.481609     2.053772      30.26
 C      -5.136977    -3.446764     0.065708      86.48
 O      -4.975242    -4.383660    -1.060758     258.08
 H      -4.910115    -5.342260    -0.845290      30.24
 H      -5.960825    -2.766895    -0.151765      28.45
 H      -5.339131    -3.930308     1.215537      26.21
55
name = lig-etoh-frame_295
 C       3.203005     2.217900    -1.996373      64.77
 H       3.134779     3.179376    -2.471674      21.65
 C       3.533838     1.307865     0.395544      54.37
 H       3.654464     1.455222     1.426213      22.65
 C       4.136130     0.110049    -0.370192      20.57
 O       4.729709    -0.979173     0.147412     210.88
 C       5.449600    -0.877595     1.463560     112.52
 H       4.866136    -0.671245     2.397275      26.62
 H       6.273568    -0.193720     1.252890      27.72
 H       5.805622    -1.904193     1.531877      26.97
 C       3.987064     0.043043    -1.760324      23.28
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 O       4.172051    -1.203069    -2.389129     231.38
 H       4.773576    -1.657482    -1.763803      26.05
 C       3.557237     1.086901    -2.582174      47.69
 H       3.162296     0.955499    -3.656626      21.41
 C       2.974261     2.292160    -0.501571      38.56
 C       2.326546     3.574594     0.098943     117.46
 H       2.525411     4.444857    -0.373291      24.63
 O       2.623875     3.843785     1.501947     278.53
 H       3.544292     4.311787     1.751926      26.86
 C       0.840769     3.522531     0.096661      77.64
 H       0.373587     3.379867    -0.892638      22.08
 C       0.211338     4.836089     0.562450     106.80
 O       0.542695     6.007477    -0.222409     146.05
 H      -0.002722     5.868369    -1.165593      26.24
 H       0.489979     4.997451     1.493255      28.08
 H      -0.952952     4.685677     0.427903      23.77
 C      -1.218453    -0.654558    -0.313661      51.59
 H      -1.145394    -1.690452    -0.088135      22.28
 C      -3.006071     0.949798    -0.325415      67.86
 H      -4.064865     1.085373     0.027786      24.55
 C      -2.271872     1.864934     0.395356      -3.76
 O      -2.439018     3.080295     0.980410     213.12
 C      -3.861537     3.224484     1.134648     142.63
 H      -4.302713     3.012696     0.229365      28.83
 H      -4.194223     2.614211     1.887321      29.83
 H      -4.061770     4.109415     1.492814      30.42
 C      -0.705495     1.610626     0.397068      -0.59
 O       0.327607     2.421062     0.941919     175.88
 C      -0.258870     0.363458     0.101259      36.96
 H       0.859675    -0.000338     0.398873      19.40
 C      -2.503030    -0.430988    -0.610429      14.90
 C      -3.505515    -1.600832    -0.880014      84.44
 H      -4.427677    -1.111620    -1.440421      22.86
 O      -2.860259    -2.359374    -2.073832     235.55
 H      -3.012485    -3.255368    -1.693334      26.38
 C      -3.877196    -2.436573     0.185533     119.08
 H      -3.038581    -2.847257     0.801172      23.42
 O      -4.371744    -1.510211     1.291460     252.91
 H      -3.877714    -1.582876     2.291630      23.98
 C      -5.034215    -3.491388     0.030723     111.09
 O      -4.994286    -4.316599    -0.990537     308.19
 H      -4.879941    -5.167785    -0.637783      32.34
 H      -5.926855    -2.772647    -0.113251      27.71
 H      -5.252834    -3.922175     0.907166      30.22
55
name = lig-etoh-frame_296
 C       3.173540     2.253956    -1.956428      27.52
 H       2.857623     3.185601    -2.491086      18.91
 C       3.511034     1.267600     0.383871      76.39
 H       3.994966     1.864144     1.338433      21.80
 C       4.122443     0.165141    -0.398936      13.62
 O       4.672878    -0.960698     0.140865     222.28
 C       5.436118    -0.891315     1.447580     106.10
 H       4.774295    -0.484485     2.308025      25.14
 H       6.217442    -0.094712     1.344920      27.09
 H       6.078829    -1.782395     1.807543      25.58
 C       4.008420    -0.010337    -1.800430      13.19
 O       4.166764    -1.172941    -2.306554     190.49
 H       4.937237    -1.808177    -1.933980      21.83
 C       3.564209     1.053738    -2.580346      54.04
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 H       3.518842     0.916637    -3.654362      25.02
 C       2.892852     2.295398    -0.486410      54.94
 C       2.387130     3.596881     0.079351     100.23
 H       2.292668     4.593464    -0.721547      23.98
 O       2.615889     3.806164     1.471565     297.53
 H       3.507305     4.144666     1.543555      29.78
 C       0.830499     3.513650     0.060322      66.78
 H       0.513431     3.398591    -1.026423      22.19
 C       0.230205     4.890845     0.518974     109.54
 O       0.549587     5.963254    -0.254629     201.40
 H       0.204584     6.084444    -1.117760      30.23
 H       0.700170     5.014063     1.668382      24.21
 H      -0.911788     4.674133     0.484149      24.72
 C      -1.237947    -0.630136    -0.279518      40.93
 H      -0.967729    -1.742848    -0.310048      22.09
 C      -3.068550     0.885551    -0.296036      61.99
 H      -4.163705     0.857816    -0.363354      25.52
 C      -2.180534     1.860048     0.364698      -9.81
 O      -2.470213     3.052543     0.957134     146.95
 C      -3.940518     3.202008     1.170704      92.33
 H      -4.303711     3.086567    -0.020951      22.86
 H      -4.406225     2.579110     2.082080      24.57
 H      -4.054092     4.356942     1.662150      24.24
 C      -0.636903     1.572281     0.385645      -2.08
 O       0.278962     2.464724     0.962864     188.32
 C      -0.206855     0.313733     0.073385      49.65
 H       0.674055     0.027050     0.445905      23.82
 C      -2.606960    -0.353356    -0.596937      28.10
 C      -3.497650    -1.498474    -0.921538      87.71
 H      -4.260791    -1.033649    -1.445128      25.93
 O      -2.933745    -2.398367    -2.038670     246.57
 H      -3.163148    -3.293507    -1.850773      28.00
 C      -3.822692    -2.438233     0.280360     104.24
 H      -2.839828    -2.743306     0.652415      25.91
 O      -4.296684    -1.461436     1.288745     318.55
 H      -3.747099    -1.777160     2.001775      29.09
 C      -4.961827    -3.401212     0.044372      96.54
 O      -5.002444    -4.316143    -0.995558     253.65
 H      -4.742164    -5.167632    -0.480156      27.79
 H      -5.914173    -2.827721    -0.057981      26.83
 H      -5.112292    -4.102235     1.084501      25.06
55
name = lig-etoh-frame_297
 C       3.091277     2.307817    -1.858812      66.94
 H       2.622893     2.993173    -2.573503      23.15
 C       3.519002     1.271831     0.310354      92.35
 H       4.012485     1.699310     1.064558      26.05
 C       4.086723     0.261302    -0.371421       4.70
 O       4.656056    -0.977879     0.185147     229.96
 C       5.427032    -0.854617     1.428098     125.36
 H       4.688316    -0.486079     2.127078      26.49
 H       6.115234    -0.004731     1.388310      28.00
 H       5.973004    -1.683847     1.777364      28.07
 C       4.002670     0.010374    -1.786265      15.50
 O       4.191182    -1.235035    -2.278785     209.81
 H       4.931848    -1.739556    -2.015699      25.79
 C       3.571259     1.041683    -2.593226      55.34
 H       3.870014     0.926789    -3.676494      24.65
 C       2.901911     2.295005    -0.512360      53.37
 C       2.365403     3.620806     0.035613     109.93
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 H       2.597569     4.331583    -0.640675      30.87
 O       2.634420     3.777926     1.439202     299.61
 H       3.660807     3.971372     1.402517      26.12
 C       0.794289     3.517786     0.002008      69.46
 H       0.614066     3.252793    -1.017094      25.05
 C       0.228250     4.875811     0.523834     118.48
 O       0.593420     5.979305    -0.296978     200.34
 H       0.265410     5.975648    -1.213135      29.84
 H       0.569970     5.118154     1.420529      28.95
 H      -0.916812     4.750728     0.689988      25.61
 C      -1.231776    -0.652781    -0.264065      54.00
 H      -0.722719    -1.564555    -0.612804      22.82
 C      -3.145609     0.890147    -0.226693      43.95
 H      -4.184447     0.979663    -0.705893      19.49
 C      -2.013974     1.817591     0.302424       0.53
 O      -2.533758     3.024408     0.948783     134.52
 C      -4.010162     3.232433     1.208454     129.96
 H      -4.517371     3.224198     0.346483      29.79
 H      -4.439457     2.474154     1.791079      28.64
 H      -4.026324     4.193550     1.454260      29.84
 C      -0.643339     1.576690     0.384851      20.59
 O       0.225686     2.517466     0.975027     188.90
 C      -0.224241     0.224708     0.045704      20.21
 H       0.921752    -0.086359     0.459310      20.63
 C      -2.608992    -0.322232    -0.566187      23.78
 C      -3.480961    -1.432339    -1.024109      61.73
 H      -4.551712    -0.984400    -1.382615      25.51
 O      -2.992081    -2.418158    -1.995503     213.94
 H      -3.439222    -3.368660    -2.003003      22.22
 C      -3.759525    -2.375522     0.371206      83.95
 H      -2.743901    -2.904614     0.404357      26.54
 O      -4.225090    -1.434937     1.290287     307.77
 H      -3.616811    -1.679904     2.079862      25.94
 C      -4.941217    -3.309872     0.155747      98.38
 O      -4.989696    -4.365325    -1.033730     229.54
 H      -4.546964    -5.176533    -0.641428      30.17
 H      -5.858230    -2.731907     0.067887      28.86
 H      -4.887964    -3.890990     0.997610      29.49
55
name = lig-etoh-frame_298
 C       3.003280     2.274768    -1.872447      86.41
 H       2.469015     2.951569    -2.539987      23.74
 C       3.526370     1.335638     0.221497      67.99
 H       3.956084     1.481132     1.376615      21.19
 C       4.078575     0.235613    -0.352913      20.63
 O       4.658359    -0.984416     0.234501     235.81
 C       5.391364    -0.757900     1.408519     113.49
 H       4.558420    -0.608573     2.254996      24.34
 H       6.130969     0.081492     1.330514      26.31
 H       5.795868    -1.826912     1.623767      25.12
 C       3.981515     0.048941    -1.744071      14.27
 O       4.216475    -1.316757    -2.289321     146.24
 H       5.055528    -1.702303    -1.864286      23.22
 C       3.580598     1.089087    -2.580399      62.81
 H       3.975892     1.097622    -3.623900      25.87
 C       2.943542     2.321912    -0.526814      41.48
 C       2.290213     3.571436     0.029169     104.35
 H       3.008965     4.446470    -0.577662      23.01
 O       2.695388     3.767361     1.398197     301.76
 H       3.712916     3.815328     1.517571      25.95
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 C       0.759618     3.543871    -0.034326      70.30
 H       0.424004     3.118800    -1.069181      22.54
 C       0.189425     4.834090     0.490244      94.23
 O       0.645792     6.027058    -0.353673     134.55
 H       0.305697     5.592903    -1.303102      26.89
 H       0.680127     5.194702     1.558940      23.16
 H      -0.947618     4.914769     0.819469      23.72
 C      -1.198737    -0.710174    -0.298403      54.93
 H      -0.809826    -1.583927    -0.814029      22.89
 C      -3.143071     0.929107    -0.168582      49.53
 H      -3.976763     1.435971    -0.642067      18.94
 C      -1.992051     1.807325     0.253155      -4.01
 O      -2.591847     2.992723     0.936347      99.06
 C      -4.022837     3.231981     1.209063      92.10
 H      -4.903396     3.322168     0.283429      23.69
 H      -4.457348     2.308587     1.791042      24.45
 H      -4.041504     4.391553     1.639932      23.69
 C      -0.644185     1.561866     0.388963      23.05
 O       0.181083     2.565383     0.970303     184.55
 C      -0.220951     0.188614     0.076273      43.02
 H       0.708926    -0.122755     0.117022      24.20
 C      -2.555880    -0.344056    -0.552443      -0.58
 C      -3.527508    -1.432712    -1.105624      84.34
 H      -4.508842    -1.123956    -1.207860      28.08
 O      -3.028325    -2.428081    -1.973743     251.46
 H      -3.804385    -3.047354    -1.941498      24.51
 C      -3.691010    -2.273684     0.338652      87.96
 H      -2.864893    -2.956457     0.444274      27.11
 O      -4.135519    -1.427653     1.338134     291.12
 H      -3.676207    -1.211063     2.296333      24.21
 C      -4.919746    -3.262459     0.239881      66.50
 O      -4.960861    -4.392273    -1.053913     196.12
 H      -4.397583    -5.096967    -0.809656      30.95
 H      -5.910493    -2.620510     0.169040      27.08
 H      -4.889608    -3.913738     1.254095      26.25
55
name = lig-etoh-frame_299
 C       2.925397     2.183903    -1.996400      43.60
 H       2.427855     3.056710    -2.471677      23.16
 C       3.593043     1.397940     0.246935      67.28
 H       3.418535     1.282615     1.267433      24.09
 C       4.083811     0.119943    -0.364751      25.55
 O       4.645438    -0.953266     0.256230     238.83
 C       5.331928    -0.691701     1.441534     132.41
 H       4.759148    -0.587935     2.334911      28.37
 H       6.127820     0.042086     1.345143      28.03
 H       5.759512    -1.646063     1.535902      28.31
 C       3.968460     0.021089    -1.739326      20.60
 O       4.252078    -1.352059    -2.298494     138.01
 H       5.039153    -1.656363    -1.662895      23.06
 C       3.593308     1.169511    -2.539714      47.34
 H       3.778560     1.234802    -3.593942      20.63
 C       2.962487     2.373439    -0.533385      34.63
 C       2.294483     3.539573     0.031811     116.30
 H       2.689962     4.360690    -0.382788      24.83
 O       2.751445     3.754736     1.385699     342.01
 H       3.682873     3.794883     1.447773      29.83
 C       0.705734     3.556391    -0.060513      78.45
 H       0.273186     3.302740    -0.968869      24.26
 C       0.168724     4.883784     0.495812     111.13
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 O       0.667408     6.023497    -0.433487     198.48
 H       0.581969     5.636273    -1.265994      33.43
 H       0.751018     4.912056     1.372122      26.09
 H      -0.915209     4.904067     0.617866      25.66
 C      -1.178410    -0.768908    -0.376363      34.68
 H      -1.014686    -1.791047    -0.845382      22.56
 C      -3.009693     0.947786    -0.149819      60.94
 H      -3.835338     1.684012    -0.401340      19.75
 C      -2.127486     1.835785     0.256590       1.94
 O      -2.626443     2.976923     0.908693     172.81
 C      -4.053571     3.232215     1.180849     131.63
 H      -4.582545     3.389121     0.373097      29.70
 H      -4.363887     2.487115     1.871818      28.37
 H      -4.041216     3.995420     1.899136      28.37
 C      -0.619938     1.523962     0.404513       7.41
 O       0.148289     2.592770     0.953347     192.92
 C      -0.243769     0.216767     0.121463      51.33
 H       0.915137    -0.162400    -0.168128      21.56
 C      -2.551056    -0.365739    -0.577071       4.80
 C      -3.537309    -1.451375    -1.069560      85.39
 H      -4.639553    -1.050496    -1.330540      24.47
 O      -3.071954    -2.431827    -1.979432     249.33
 H      -3.936563    -2.909158    -2.001510      24.57
 C      -3.660783    -2.202522     0.264809      91.45
 H      -2.771625    -2.805174     0.605789      25.26
 O      -4.072375    -1.386164     1.410727     334.09
 H      -3.527597    -1.248375     2.147648      31.25
 C      -4.903316    -3.257603     0.311008      80.22
 O      -4.936699    -4.368275    -1.043284     153.41
 H      -4.135769    -5.004915    -0.826177      27.32
 H      -5.805108    -2.779660     0.178176      29.45
 H      -5.005768    -3.847691     1.223331      27.83
55
name = lig-etoh-frame_300
 C       2.831633     2.176520    -2.035799      56.30
 H       2.529500     3.033445    -2.632409      25.20
 C       3.660427     1.386851     0.268021      60.03
 H       3.026860     1.303207     1.293305      22.24
 C       4.055987     0.087790    -0.389794       9.97
 O       4.612479    -0.921474     0.271807     222.14
 C       5.308088    -0.660841     1.499307     105.99
 H       4.770280    -0.359588     2.531483      24.57
 H       6.102832     0.127164     1.358934      26.03
 H       5.990141    -1.577313     1.689158      26.01
 C       3.971803    -0.056730    -1.781621      20.24
 O       4.299500    -1.325544    -2.291040     225.74
 H       4.861880    -1.739730    -1.690867      26.44
 C       3.622983     1.172750    -2.537531      46.20
 H       3.510569     1.136281    -3.695743      21.01
 C       2.980869     2.365563    -0.590232      22.38
 C       2.294617     3.519837     0.057583      87.93
 H       2.378775     4.649400    -0.657250      19.66
 O       2.774570     3.736327     1.407673     240.85
 H       3.835101     3.895370     1.241248      23.66
 C       0.654417     3.562045    -0.039514      56.29
 H       0.228800     3.458134    -1.142433      21.12
 C       0.198598     4.960283     0.461494      98.24
 O       0.678144     5.991911    -0.486289     147.72
 H       0.791285     5.706849    -1.489809      26.18
 H       0.733962     4.939759     1.495048      23.21
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 H      -1.033621     4.868752     0.371468      23.18
 C      -1.211160    -0.791305    -0.470385      40.48
 H      -0.970158    -1.815587    -0.654287      23.95
 C      -2.903839     0.917616    -0.205861      60.48
 H      -3.984973     1.196628    -0.235658      24.26
 C      -2.166438     1.896287     0.350289      13.66
 O      -2.634338     2.993637     0.877505     194.84
 C      -4.030969     3.201860     1.200727     102.81
 H      -4.560232     3.542283     0.090040      23.44
 H      -4.497773     2.338172     1.822579      25.26
 H      -3.994180     4.021726     2.052529      24.74
 C      -0.662338     1.522089     0.435561      -8.87
 O       0.124120     2.592428     0.923750     184.98
 C      -0.223205     0.208723     0.115406      49.20
 H       0.771302     0.119272    -0.086304      24.66
 C      -2.542218    -0.377029    -0.630783      18.60
 C      -3.558593    -1.436444    -0.971848      96.92
 H      -4.364407    -0.971373    -1.458068      25.18
 O      -3.119119    -2.427329    -2.007837     220.10
 H      -3.875012    -3.122184    -2.245592      22.37
 C      -3.691911    -2.200089     0.271847      95.49
 H      -2.660054    -2.504549     0.506524      24.60
 O      -4.050316    -1.326622     1.439305     280.02
 H      -3.149021    -1.564836     2.118536      22.93
 C      -4.858720    -3.278538     0.317590      78.18
 O      -4.900470    -4.314566    -0.989335     197.78
 H      -4.017747    -4.737693    -0.821159      28.91
 H      -5.940284    -2.791051     0.048398      24.76
 H      -4.932611    -3.914818     1.257330      26.22
55
name = lig-etoh-frame_301
 C       2.790131     2.215263    -1.999872      71.74
 H       2.557520     2.925581    -2.827905      25.17
 C       3.660493     1.337142     0.242538      74.57
 H       3.141374     1.405418     1.181822      22.79
 C       4.004610     0.165831    -0.405411       4.37
 O       4.585689    -0.927226     0.320353     215.43
 C       5.338301    -0.626838     1.587834     113.21
 H       4.693822    -0.290931     2.328054      27.15
 H       5.920951     0.256565     1.330562      26.57
 H       5.972552    -1.436312     1.876133      27.68
 C       3.980795    -0.099905    -1.830772      14.71
 O       4.342987    -1.272369    -2.306974     198.70
 H       4.807079    -1.927668    -1.637965      21.70
 C       3.621084     1.076069    -2.601931      51.22
 H       3.483470     0.879641    -3.613889      23.54
 C       2.992402     2.326813    -0.651874      31.04
 C       2.262807     3.567827     0.041785     102.78
 H       2.304017     4.291438    -0.590495      26.10
 O       2.803838     3.724083     1.415665     278.20
 H       3.707193     4.041744     1.275933      29.03
 C       0.633917     3.563219    -0.009382      67.69
 H       0.423345     3.425368    -1.017052      23.48
 C       0.227218     5.000741     0.385818     118.17
 O       0.693249     5.963087    -0.523941     227.64
 H       0.809822     5.638072    -1.527368      26.41
 H       0.385446     5.380555     1.454535      24.03
 H      -0.806662     5.002086     0.416039      26.60
 C      -1.204152    -0.758387    -0.531946      58.30
 H      -0.769168    -1.806905    -0.497362      23.06
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 C      -2.910544     0.867008    -0.292715      45.92
 H      -4.005117     0.551988    -0.155524      21.80
 C      -2.088059     1.882944     0.446912      13.62
 O      -2.633532     3.059527     0.872697     213.85
 C      -4.017770     3.179000     1.220471     133.93
 H      -4.498896     3.549737     0.445064      30.12
 H      -4.565863     2.257609     1.377648      27.26
 H      -4.006709     4.079668     1.836385      26.75
 C      -0.763265     1.549973     0.469487      11.57
 O       0.105561     2.570704     0.891397     197.78
 C      -0.265329     0.209921     0.068490      15.14
 H       0.966264     0.219587     0.090757      21.18
 C      -2.488817    -0.395279    -0.696486      14.16
 C      -3.578713    -1.416808    -0.930408      75.51
 H      -4.437406    -0.815922    -1.420688      23.37
 O      -3.146682    -2.417015    -2.051231     231.41
 H      -3.752482    -3.103349    -2.215836      27.38
 C      -3.774261    -2.226912     0.350897      93.50
 H      -2.694155    -2.533795     0.341999      25.92
 O      -4.007745    -1.279731     1.450102     328.88
 H      -3.444204    -1.654133     2.158336      28.23
 C      -4.844275    -3.311947     0.255985     108.74
 O      -4.845140    -4.236515    -0.896905     285.74
 H      -3.978880    -4.598710    -0.848216      32.58
 H      -5.710862    -2.823079     0.159883      28.37
 H      -4.735822    -3.943655     1.224040      26.74
55
name = lig-etoh-frame_302
 C       2.860566     2.182193    -2.024143     109.04
 H       2.399286     2.881496    -2.742336      26.19
 C       3.589502     1.333377     0.154157      52.48
 H       3.504102     1.435838     1.320187      19.75
 C       3.998906     0.197792    -0.399300      17.44
 O       4.562743    -0.948100     0.380261     211.49
 C       5.357966    -0.557872     1.631714      99.93
 H       4.416445    -0.289799     2.345286      23.43
 H       5.886785     0.390189     1.367628      25.40
 H       5.923085    -1.449440     2.016047      25.73
 C       3.979584    -0.046328    -1.834156      23.49
 O       4.401441    -1.255168    -2.352753     166.60
 H       4.693274    -1.886701    -1.597694      22.76
 C       3.552584     0.951784    -2.648752      64.80
 H       3.551933     0.672817    -3.790386      20.58
 C       2.965357     2.327710    -0.650785      35.38
 C       2.228259     3.540733     0.047458      93.68
 H       2.626955     4.548737    -0.747745      19.56
 O       2.807881     3.724055     1.400347     267.03
 H       3.735307     4.174336     1.421661      26.56
 C       0.683153     3.562022     0.060269      61.64
 H       0.454451     3.266797    -1.062640      20.01
 C       0.220673     5.029060     0.326329     106.71
 O       0.729228     5.955295    -0.582610     225.64
 H       0.620011     5.535834    -1.405551      32.41
 H       0.364429     5.603565     1.276517      23.07
 H      -1.035088     5.109308     0.390095      22.54
 C      -1.063984    -0.721726    -0.541142      66.83
 H      -0.705620    -1.724328    -0.582637      23.79
 C      -2.957189     0.830915    -0.337958      45.23
 H      -3.975996     0.617142    -0.026291      23.21
 C      -2.118106     1.797335     0.476787       0.28
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 O      -2.603430     3.128105     0.879393     178.23
 C      -4.003262     3.165759     1.222373     108.38
 H      -4.676633     3.717281     0.248150      24.33
 H      -4.506828     2.168247     1.294424      25.71
 H      -4.126998     3.992049     1.998948      25.07
 C      -0.798845     1.562897     0.478357      21.97
 O       0.096450     2.538854     0.880653     208.62
 C      -0.318627     0.264286     0.003737      43.01
 H       0.697639     0.067117     0.320299      22.15
 C      -2.448478    -0.416109    -0.768549     -12.41
 C      -3.609856    -1.406685    -0.971760      70.64
 H      -4.551621    -0.872646    -1.151033      24.19
 O      -3.149142    -2.371957    -2.083617     208.49
 H      -3.893623    -3.055780    -2.046038      24.56
 C      -3.822743    -2.231048     0.409861      84.41
 H      -2.889642    -2.871755     0.458181      24.76
 O      -3.989192    -1.256538     1.434551     286.48
 H      -3.607368    -1.533574     2.494980      21.24
 C      -4.820211    -3.357360     0.225016      98.51
 O      -4.781572    -4.157316    -0.807573     272.21
 H      -3.864561    -4.650157    -0.889180      29.24
 H      -5.892505    -2.745944     0.353074      25.86
 H      -4.703815    -3.934916     1.145392      28.46
55
name = lig-etoh-frame_303
 C       2.981463     2.084494    -2.103309      52.00
 H       2.300370     2.835488    -2.546761      18.89
 C       3.476249     1.372381     0.124512      51.24
 H       4.061923     1.524888     1.089641      21.75
 C       4.046348     0.130978    -0.398978      12.56
 O       4.548541    -0.951890     0.430629     233.27
 C       5.295860    -0.473483     1.655614     119.85
 H       4.604577    -0.336248     2.387905      27.85
 H       5.981262     0.359664     1.546355      28.13
 H       5.856994    -1.349914     2.023571      27.73
 C       3.994218    -0.012220    -1.791931      15.44
 O       4.460995    -1.245594    -2.398452     217.83
 H       4.667551    -1.736912    -1.651850      25.89
 C       3.424712     0.884743    -2.710808      58.78
 H       3.567590     0.708606    -3.720884      27.72
 C       2.899380     2.352932    -0.635840      47.63
 C       2.279297     3.543462     0.029204     121.68
 H       2.633898     4.325620    -0.374341      27.02
 O       2.790662     3.727452     1.380740     313.09
 H       3.727699     4.196535     1.428847      26.33
 C       0.747637     3.558129     0.085040      65.00
 H       0.409130     3.290022    -0.878342      22.66
 C       0.128092     5.063822     0.311770     103.51
 O       0.775752     5.952491    -0.666743     189.86
 H       0.403776     5.548800    -1.628690      25.21
 H       0.636108     5.457112     1.307727      23.47
 H      -0.870918     5.003019     0.184121      26.38
 C      -0.966839    -0.707211    -0.564364      39.06
 H      -0.587026    -1.725057    -0.787890      21.57
 C      -2.987422     0.809701    -0.316323      44.88
 H      -4.075749     1.067932    -0.071260      21.64
 C      -2.255434     1.737431     0.444818     -17.66
 O      -2.564427     3.150274     0.885698     186.57
 C      -4.027295     3.206299     1.163315     128.96
 H      -4.479713     3.611753     0.414324      29.56
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 H      -4.331749     2.185238     1.463845      26.68
 H      -4.263296     3.559815     2.238041      25.90
 C      -0.774206     1.563784     0.449206      11.98
 O       0.105830     2.508460     0.913699     188.49
 C      -0.333752     0.364129    -0.014454      58.73
 H       0.656185    -0.027482     0.398747      22.13
 C      -2.436386    -0.421708    -0.822861     -10.99
 C      -3.589346    -1.427644    -1.013239      74.26
 H      -4.631781    -0.976203    -1.108390      24.11
 O      -3.174374    -2.310023    -2.099309     220.12
 H      -3.966379    -2.971355    -1.962337      22.54
 C      -3.794865    -2.236961     0.422847      91.26
 H      -2.986237    -2.925491     0.702421      24.29
 O      -3.990983    -1.248784     1.426613     346.51
 H      -3.713251    -1.328470     2.391565      25.90
 C      -4.872592    -3.313393     0.337512     108.44
 O      -4.707577    -4.130793    -0.809000     290.05
 H      -3.891570    -4.668958    -0.745913      30.78
 H      -5.858034    -3.049799     0.328891      29.21
 H      -4.774047    -4.012234     1.291976      27.80
55
name = lig-etoh-frame_304
 C       3.033848     2.030663    -2.147350      53.11
 H       2.396720     2.765823    -2.694633      20.82
 C       3.455491     1.351908     0.140320      43.23
 H       4.055077     1.750009     0.949240      21.81
 C       4.069378     0.088043    -0.394159       9.73
 O       4.548351    -0.919113     0.472990     239.52
 C       5.225899    -0.426535     1.664841     111.47
 H       4.576811    -0.173102     2.666160      24.22
 H       6.037229     0.356320     1.597652      26.71
 H       5.855009    -1.293001     1.925135      26.91
 C       4.026203    -0.067673    -1.778713      11.63
 O       4.511850    -1.206900    -2.433827     183.13
 H       4.841192    -1.860198    -1.654598      21.74
 C       3.308263     0.860225    -2.719548      56.36
 H       3.463324     0.749758    -3.854777      24.89
 C       2.853076     2.327532    -0.681177      30.38
 C       2.345566     3.535265     0.052149      97.46
 H       2.635366     4.698537    -0.558054      20.03
 O       2.771661     3.727371     1.386858     308.78
 H       3.635479     4.065295     1.294707      29.41
 C       0.766921     3.567856     0.078188      51.57
 H       0.376246     3.343440    -0.977368      20.67
 C       0.135618     5.071457     0.316986      93.16
 O       0.795284     5.924095    -0.773583     175.02
 H       0.499286     5.836348    -1.675482      28.64
 H       0.492416     5.245820     1.270372      26.08
 H      -1.090560     4.922517     0.115998      22.51
 C      -1.016756    -0.693501    -0.630118      29.53
 H      -0.424290    -1.590468    -0.925347      19.53
 C      -3.036942     0.808189    -0.250135      62.88
 H      -4.032220     1.233770    -0.576217      21.38
 C      -2.280970     1.757795     0.389589      -1.63
 O      -2.553842     3.116594     0.887906     181.61
 C      -4.015004     3.203449     1.180653     109.62
 H      -4.638706     3.772769     0.203475      24.00
 H      -4.296272     2.145024     1.336924      27.21
 H      -4.240510     3.544273     2.158048      27.29
 C      -0.817342     1.602802     0.407248       6.93
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 O       0.135179     2.493124     0.986471     157.33
 C      -0.256657     0.410417    -0.002277      25.88
 H       0.856402     0.173515     0.326205      20.46
 C      -2.435924    -0.413912    -0.831803       7.32
 C      -3.522887    -1.463716    -1.021260      80.99
 H      -4.519428    -1.016855    -1.258691      23.96
 O      -3.229720    -2.256094    -2.109994     266.60
 H      -3.803754    -2.996611    -2.116890      26.67
 C      -3.739886    -2.244560     0.434665      74.36
 H      -2.767179    -2.739991     0.803188      23.44
 O      -4.040553    -1.213448     1.381211     278.85
 H      -3.445505    -1.492666     2.305571      22.14
 C      -4.933711    -3.287337     0.508461      82.80
 O      -4.634482    -4.132666    -0.847308     275.32
 H      -3.908265    -4.668531    -0.524622      30.46
 H      -6.104278    -3.072484     0.240576      25.55
 H      -4.854892    -3.918689     1.346282      28.91
55
name = lig-etoh-frame_305
 C       2.963064     2.083323    -2.144164      44.45
 H       2.681802     2.744517    -3.001083      19.24
 C       3.502657     1.295827     0.137224      50.87
 H       3.690879     1.908964     1.155459      18.00
 C       4.044468     0.108962    -0.379726      11.36
 O       4.555556    -0.860015     0.508309     240.37
 C       5.181239    -0.402677     1.718091     119.98
 H       4.585744    -0.058050     2.475777      27.62
 H       5.847249     0.414079     1.422622      27.69
 H       5.807877    -1.306745     1.934383      26.50
 C       4.030368    -0.156241    -1.820113      14.14
 O       4.570991    -1.179533    -2.443796     209.94
 H       5.049347    -1.927100    -1.995817      23.21
 C       3.280518     0.785172    -2.690429      53.74
 H       3.224014     0.714767    -3.774709      24.90
 C       2.870655     2.242112    -0.750535      42.15
 C       2.372325     3.604870     0.027109     101.28
 H       2.435279     4.341804    -0.581155      26.50
 O       2.757704     3.720690     1.406450     273.98
 H       3.807929     3.982053     1.330755      25.99
 C       0.738930     3.580559     0.033478      51.33
 H       0.486364     3.319691    -1.007935      21.33
 C       0.159100     5.013265     0.244385     100.39
 O       0.808786     5.902705    -0.824019     216.69
 H       0.462585     5.792260    -1.776967      26.80
 H       0.270958     5.439029     1.418861      23.75
 H      -0.827284     5.033217     0.303807      26.87
 C      -1.091144    -0.611970    -0.682920      49.58
 H      -0.523344    -1.444044    -0.974811      22.64
 C      -3.087466     0.819009    -0.227155      60.40
 H      -3.920828     1.011656    -0.924313      20.90
 C      -2.197652     1.855922     0.338466      14.18
 O      -2.583781     3.049826     0.885146     200.58
 C      -4.006570     3.180151     1.167190     118.62
 H      -4.525639     3.719974     0.498934      28.88
 H      -4.465921     2.175426     1.031226      25.66
 H      -4.110839     3.929736     2.093868      24.88
 C      -0.850322     1.638476     0.378190      -4.72
 O       0.166074     2.505989     1.059939     112.27
 C      -0.177434     0.389802    -0.013676      12.63
 H       0.904907     0.465070     0.103353      21.01
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 C      -2.442890    -0.393940    -0.786483      16.60
 C      -3.470664    -1.498224    -0.997977      80.27
 H      -4.403238    -0.909065    -1.232233      23.66
 O      -3.257858    -2.225139    -2.161475     250.76
 H      -3.701412    -3.158574    -2.173201      21.68
 C      -3.705119    -2.239027     0.444905      88.44
 H      -2.705470    -2.597089     0.645068      24.83
 O      -4.091894    -1.176021     1.366234     321.95
 H      -3.282245    -1.410009     1.896447      25.89
 C      -4.979581    -3.270492     0.581442      68.43
 O      -4.569532    -4.144641    -0.853856     212.40
 H      -3.896599    -4.760889    -0.319826      25.72
 H      -5.904354    -2.809838     0.289926      26.74
 H      -4.926783    -3.967399     1.563044      25.43
55
name = lig-etoh-frame_306
 C       2.852001     2.107744    -2.165045      73.17
 H       2.918242     2.851860    -2.994417      20.75
 C       3.533317     1.294614     0.121161      64.14
 H       3.316085     1.475744     1.141612      21.04
 C       4.017236     0.127393    -0.364441       7.04
 O       4.555495    -0.811008     0.519007     214.28
 C       5.182567    -0.384651     1.736987     106.43
 H       4.326501     0.031094     2.498144      23.63
 H       5.735940     0.512749     1.364313      25.40
 H       5.727447    -1.216161     2.175837      26.21
 C       3.977245    -0.190655    -1.839373      19.65
 O       4.653718    -1.198174    -2.488225     226.18
 H       5.163319    -1.882862    -2.096103      25.11
 C       3.300850     0.721163    -2.609498      60.50
 H       3.098236     0.510113    -3.680429      22.45
 C       2.921337     2.201001    -0.774594      56.57
 C       2.320268     3.583413    -0.005644      93.54
 H       2.575659     4.576343    -0.852653      19.71
 O       2.784111     3.725876     1.409278     287.45
 H       3.715747     3.920436     1.562415      28.87
 C       0.726046     3.576060     0.007292      51.07
 H       0.485489     3.181719    -1.006983      21.10
 C       0.223821     4.969669     0.185914     112.85
 O       0.809558     5.883775    -0.832496     192.34
 H       0.377256     5.456565    -1.721949      24.91
 H       0.424700     5.524743     1.001312      25.42
 H      -1.005819     5.023136     0.096938      22.80
 C      -1.073239    -0.485673    -0.690876      52.21
 H      -0.784227    -1.548148    -1.076128      22.16
 C      -3.067405     0.843799    -0.253244      48.21
 H      -4.009340     0.925854    -0.901182      19.14
 C      -2.156451     1.932443     0.265738      14.43
 O      -2.633791     2.998146     0.886110     194.42
 C      -3.990532     3.167287     1.173646     111.72
 H      -4.527130     3.960988     0.253242      23.66
 H      -4.637531     2.286877     1.142533      25.83
 H      -3.966362     3.817272     1.956087      27.44
 C      -0.754486     1.623468     0.379862      -0.22
 O       0.178368     2.547993     1.089736     130.90
 C      -0.205178     0.390448    -0.057621      41.95
 H       0.979585     0.589100    -0.266659      19.92
 C      -2.478759    -0.355757    -0.692820       9.52
 C      -3.473661    -1.501957    -0.968049      71.99
 H      -4.396792    -0.857336    -1.014168      24.27
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 O      -3.255635    -2.226166    -2.251837     246.26
 H      -3.605428    -3.123517    -1.947358      21.61
 C      -3.734323    -2.223954     0.425850      93.43
 H      -2.700685    -2.709132     0.626449      22.92
 O      -4.120149    -1.150153     1.347076     286.00
 H      -3.395589    -0.967257     2.041137      26.21
 C      -4.914339    -3.257807     0.570277      75.29
 O      -4.517785    -4.172223    -0.796529     240.21
 H      -3.970914    -4.843796    -0.377483      29.00
 H      -5.844530    -2.545383     0.368949      26.37
 H      -5.023819    -3.833396     1.410647      28.37
55
name = lig-etoh-frame_307
 C       2.790267     2.037576    -2.187558      74.75
 H       2.799422     2.964902    -2.763932      24.19
 C       3.516567     1.320355     0.095446      63.43
 H       3.047653     0.970915     1.151078      21.28
 C       4.023089     0.094795    -0.378825       8.74
 O       4.556432    -0.802095     0.507415     215.00
 C       5.149069    -0.317538     1.753238     114.07
 H       4.358793    -0.060995     2.375543      26.26
 H       5.824208     0.546689     1.633323      26.53
 H       5.687163    -1.086472     2.381059      26.27
 C       3.938283    -0.216908    -1.783822      15.29
 O       4.729842    -1.223590    -2.557949     158.30
 H       5.215371    -1.859087    -1.818104      21.64
 C       3.293915     0.730489    -2.561394      44.31
 H       3.139830     0.257367    -3.587798      21.58
 C       2.950631     2.271588    -0.756917      37.45
 C       2.290174     3.543217    -0.075612     116.60
 H       2.692839     4.322516    -0.493387      23.24
 O       2.789306     3.730364     1.394014     295.88
 H       3.759725     3.961560     1.479571      28.25
 C       0.761478     3.532742     0.003867      46.12
 H       0.358994     3.047886    -0.951341      20.68
 C       0.227496     4.968004     0.105542     111.48
 O       0.784955     5.838455    -0.849181     276.02
 H       0.607316     5.468433    -1.701962      30.31
 H       0.762226     5.528385     1.086816      20.90
 H      -0.746187     4.883040    -0.144807      25.52
 C      -1.060011    -0.444010    -0.702123      64.28
 H      -0.908961    -1.383977    -1.072092      24.64
 C      -3.007611     0.913510    -0.314601      42.02
 H      -4.092766     1.142089    -0.421308      21.75
 C      -2.138087     1.913805     0.178412       1.77
 O      -2.665897     2.976046     0.897315     192.36
 C      -4.023762     3.212185     1.107392     120.08
 H      -4.288448     3.777132     0.360419      28.43
 H      -4.690642     2.352979     1.442477      25.99
 H      -3.993368     3.739475     2.207720      24.37
 C      -0.642651     1.628700     0.421238       1.19
 O       0.174422     2.602003     1.066234     205.61
 C      -0.210954     0.454725    -0.141296      65.60
 H       0.751239     0.314424    -0.423425      23.48
 C      -2.498128    -0.322926    -0.592972       9.98
 C      -3.509072    -1.454168    -0.951213      66.66
 H      -4.514678    -0.994724    -1.023269      23.87
 O      -3.248762    -2.232163    -2.304980     231.36
 H      -3.520142    -3.072622    -1.897834      22.84
 C      -3.734634    -2.222736     0.433534     104.77
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 H      -2.911730    -2.760595     0.785078      24.64
 O      -4.136912    -1.133330     1.330682     305.95
 H      -3.733952    -0.648116     2.156750      26.14
 C      -4.799566    -3.211122     0.441162      92.59
 O      -4.496701    -4.192012    -0.697762     289.03
 H      -3.976500    -4.950866    -0.368403      29.41
 H      -5.776081    -2.622876     0.343636      26.88
 H      -4.981750    -3.872192     1.416692      26.57
55
name = lig-etoh-frame_308
 C       2.786726     1.950710    -2.149280      75.92
 H       2.382979     2.851431    -2.725115      24.22
 C       3.452129     1.291185     0.093536      67.37
 H       3.060491     1.099693     1.001196      23.80
 C       4.046233     0.065583    -0.417104      28.12
 O       4.583994    -0.827299     0.501095     205.96
 C       5.116116    -0.246396     1.778492     103.52
 H       4.210814     0.035914     2.476192      24.71
 H       5.869022     0.569985     1.812751      26.29
 H       5.629568    -1.075256     2.252257      27.37
 C       3.949779    -0.254758    -1.722845      23.97
 O       4.783295    -1.237182    -2.577761     214.20
 H       5.079483    -1.719806    -1.814636      25.92
 C       3.260914     0.749074    -2.577549      37.33
 H       3.246394     0.348270    -3.552953      22.12
 C       2.948724     2.361179    -0.731905      28.27
 C       2.310971     3.450405    -0.075593     110.00
 H       2.802035     4.559216    -0.553460      15.58
 O       2.776920     3.724620     1.364974     263.04
 H       3.762612     4.028372     1.114420      25.37
 C       0.797115     3.471876    -0.016000      66.16
 H       0.368105     3.094491    -0.910509      22.14
 C       0.276514     4.975587     0.077699     111.57
 O       0.779872     5.812765    -0.876373     300.03
 H       0.823321     5.571936    -1.965502      20.81
 H       0.497299     5.161749     1.054631      26.38
 H      -0.931399     4.882172     0.080656      23.87
 C      -1.146159    -0.460329    -0.709337      40.95
 H      -0.627130    -1.431217    -1.147447      21.27
 C      -2.970755     1.025611    -0.374441      55.68
 H      -3.943146     1.291263     0.182688      20.22
 C      -2.080262     1.879639     0.152596       2.48
 O      -2.649402     2.958395     0.906465     158.00
 C      -4.063366     3.248680     1.133332     109.81
 H      -4.526448     3.935284     0.125160      23.66
 H      -4.629620     2.357715     1.407581      26.58
 H      -4.106525     3.773949     2.011985      27.80
 C      -0.618191     1.684963     0.462684       9.82
 O       0.171880     2.656651     1.018115     231.14
 C      -0.174536     0.533674    -0.243172      21.97
 H       0.929901    -0.029924    -0.409915      19.77
 C      -2.500256    -0.315632    -0.558383      17.55
 C      -3.540049    -1.389470    -0.940540      56.47
 H      -4.600612    -1.099340    -1.231855      22.01
 O      -3.239669    -2.218782    -2.300403     182.69
 H      -3.461071    -3.220465    -2.047652      21.05
 C      -3.679893    -2.185176     0.469842      89.11
 H      -2.772266    -2.703692     0.975361      21.77
 O      -4.196347    -1.106476     1.306139     328.97
 H      -3.686174    -0.914318     2.090613      29.30
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 C      -4.731320    -3.230366     0.312161     106.13
 O      -4.492752    -4.201230    -0.599406     313.01
 H      -3.939538    -4.985581    -0.157329      26.97
 H      -5.792434    -2.824549     0.055805      26.33
 H      -4.728539    -3.678582     1.247020      28.41
55
name = lig-etoh-frame_309
 C       2.781673     1.945102    -2.071664      74.09
 H       2.061043     2.359389    -2.809622      22.36
 C       3.381418     1.245637     0.055624      33.22
 H       3.160392     1.500941     1.252433      18.46
 C       4.061618     0.067807    -0.406785      25.37
 O       4.639146    -0.847222     0.514340     208.14
 C       5.065318    -0.200715     1.821752     106.08
 H       4.236119     0.112764     2.459653      25.28
 H       5.774749     0.641664     1.677608      26.47
 H       5.549926    -1.157617     2.128455      25.31
 C       3.980229    -0.265538    -1.787061      20.36
 O       4.790684    -1.213433    -2.541740     205.80
 H       5.161289    -1.896693    -1.911515      25.09
 C       3.255437     0.706465    -2.593226      71.56
 H       3.282554     0.633988    -3.781235      25.83
 C       2.968432     2.314885    -0.723515      33.46
 C       2.361264     3.470731    -0.031502     118.79
 H       2.408321     4.261326    -0.660409      24.60
 O       2.775980     3.708883     1.302476     317.82
 H       3.649462     4.032077     1.180177      29.20
 C       0.806491     3.450804    -0.070942      58.14
 H       0.465296     3.103122    -1.152187      20.97
 C       0.263188     4.904599     0.061812     103.49
 O       0.811370     5.837033    -0.909428     288.73
 H       0.632980     5.469238    -1.795718      29.58
 H       0.419351     5.183166     1.262405      23.24
 H      -0.753503     4.943633     0.308364      25.26
 C      -1.176552    -0.494509    -0.714260      38.55
 H      -0.596087    -1.287649    -1.043231      20.75
 C      -2.961812     1.092605    -0.389163      54.12
 H      -3.795794     1.135515     0.230363      22.11
 C      -1.994183     1.922596     0.218325       5.30
 O      -2.610775     2.964512     0.921668     155.83
 C      -4.094745     3.286812     1.109795     108.23
 H      -4.666021     3.700324     0.383859      28.39
 H      -4.628879     2.309809     1.194617      25.18
 H      -4.138739     4.118745     1.974132      24.56
 C      -0.637803     1.712457     0.434398       1.37
 O       0.179031     2.710107     0.981265     221.07
 C      -0.129058     0.552389    -0.341216       8.95
 H       0.797842     0.229360    -0.196690      21.23
 C      -2.548671    -0.294227    -0.619723       5.46
 C      -3.547602    -1.365852    -0.937373      65.70
 H      -4.489899    -0.982040    -1.232789      23.26
 O      -3.220037    -2.198781    -2.255468     240.34
 H      -3.401249    -3.116190    -2.172826      25.29
 C      -3.622853    -2.112886     0.470938      97.54
 H      -2.664782    -2.367494     0.857247      24.54
 O      -4.265453    -1.087100     1.288600     325.55
 H      -3.571876    -1.324118     2.038684      23.83
 C      -4.714222    -3.231971     0.257628      82.42
 O      -4.458492    -4.280067    -0.552990     336.32
 H      -3.917239    -4.823636    -0.010584      29.74
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 H      -5.748868    -2.901425    -0.188846      24.82
 H      -4.752676    -3.573175     1.403052      24.93
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name = lig-etoh-frame_310
 C       2.758971     1.927372    -2.042638      76.13
 H       1.940095     2.126603    -2.745535      23.08
 C       3.342635     1.190846     0.091995      75.75
 H       3.580826     1.652059     0.976003      23.60
 C       4.053356     0.066117    -0.376744       1.89
 O       4.693093    -0.834170     0.528570     198.90
 C       5.031992    -0.203223     1.830503     106.49
 H       4.164589     0.130607     2.475031      24.89
 H       5.644165     0.648906     1.514716      26.30
 H       5.556506    -1.033426     2.341666      26.02
 C       4.031472    -0.247591    -1.896324      16.55
 O       4.776112    -1.175983    -2.472540     208.25
 H       5.194125    -2.087306    -2.134246      21.14
 C       3.280124     0.658338    -2.622860      70.88
 H       3.234345     0.772319    -3.632046      28.54
 C       2.968529     2.210294    -0.729625      48.20
 C       2.354695     3.498419    -0.012819     103.66
 H       2.366216     4.410650    -0.917730      18.89
 O       2.779352     3.696267     1.248192     297.53
 H       3.770363     4.073233     1.454384      25.20
 C       0.803990     3.467258    -0.157791      72.64
 H       0.638986     3.086294    -1.102123      23.06
 C       0.265372     4.843109     0.116546     106.80
 O       0.835829     5.865569    -0.893902     170.17
 H       0.441138     5.433435    -1.807412      24.25
 H       0.731563     5.297641     0.917176      24.51
 H      -0.916704     4.876358     0.042883      22.99
 C      -1.118663    -0.470987    -0.708262      28.20
 H      -0.731504    -1.529081    -1.017152      19.29
 C      -2.920477     1.080824    -0.366851      43.99
 H      -4.052169     1.023750    -0.020090      20.52
 C      -1.999030     1.996984     0.310268      14.07
 O      -2.573600     3.026141     0.954172     153.86
 C      -4.083789     3.291964     1.110589      94.95
 H      -4.729192     3.744677     0.063109      23.63
 H      -4.585758     2.361217     1.364186      25.47
 H      -4.090758     4.063654     1.822597      26.36
 C      -0.625665     1.699037     0.336258       9.90
 O       0.183663     2.736429     0.948974     192.83
 C      -0.190715     0.562312    -0.379996      32.89
 H       1.020461     0.471040    -0.098290      17.34
 C      -2.580403    -0.221587    -0.753752      -6.05
 C      -3.525295    -1.372958    -0.952471      73.98
 H      -4.525371    -0.768650    -1.087846      23.01
 O      -3.184687    -2.146891    -2.188878     248.11
 H      -3.447624    -3.094484    -2.039481      22.55
 C      -3.641973    -2.032851     0.369200     103.66
 H      -2.541492    -2.196455     0.692713      22.57
 O      -4.297317    -1.088076     1.301972     265.73
 H      -3.870304    -1.380493     2.229927      24.48
 C      -4.714603    -3.199059     0.306349      93.91
 O      -4.393070    -4.414789    -0.542530     299.65
 H      -3.691927    -4.922248     0.035429      26.36
 H      -5.612761    -2.676399    -0.124689      27.66
 H      -5.102535    -3.470992     1.257432      28.75
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name = lig-etoh-frame_311
 C       2.726359     1.831655    -2.084004      36.70
 H       1.950013     2.452566    -2.616933      20.14
 C       3.388895     1.128473     0.151278      90.14
 H       3.945088     1.560922     1.098401      21.91
 C       4.034380     0.029683    -0.385067      10.85
 O       4.733220    -0.810718     0.531695     217.76
 C       5.010840    -0.225652     1.818999     106.28
 H       4.056180     0.085794     2.374254      24.55
 H       5.605875     0.698231     1.603500      26.43
 H       5.623068    -0.778312     2.566232      26.37
 C       4.078916    -0.204309    -1.884278      17.51
 O       4.790592    -1.175601    -2.448550     247.24
 H       4.949014    -1.998658    -2.028756      24.45
 C       3.301920     0.669407    -2.630826      52.16
 H       3.181615     0.583367    -3.818881      23.81
 C       2.897424     2.162472    -0.728400      51.34
 C       2.337973     3.521512    -0.132351     128.34
 H       2.764716     4.317736    -0.633255      24.35
 O       2.794833     3.704589     1.251076     333.44
 H       3.757001     3.988622     1.377186      28.69
 C       0.834202     3.506391    -0.184068      61.92
 H       0.599639     2.986129    -1.234908      18.50
 C       0.262262     4.851034     0.117466     106.70
 O       0.828471     5.865659    -0.866675     177.70
 H       0.554405     5.757279    -1.872199      26.05
 H       0.900441     5.302554     0.975373      22.36
 H      -0.759635     4.802365    -0.109300      24.30
 C      -1.064153    -0.453749    -0.734008      42.35
 H      -0.967403    -1.522008    -0.883612      20.20
 C      -2.920317     1.044629    -0.298860      59.89
 H      -3.956846     1.237878    -0.514589      20.61
 C      -2.086182     2.012641     0.361143       2.22
 O      -2.555979     3.139608     1.008381     181.95
 C      -4.055694     3.282921     1.056230     112.96
 H      -4.279280     3.558948     0.109412      27.33
 H      -4.540670     2.453627     1.648589      25.50
 H      -4.083061     4.105504     1.868181      25.27
 C      -0.641831     1.729897     0.240580       5.11
 O       0.183312     2.709449     0.897341     200.22
 C      -0.216469     0.553295    -0.352673      62.30
 H       0.797432     0.500482    -0.386626      20.96
 C      -2.494780    -0.135840    -0.896578      -1.29
 C      -3.530230    -1.304267    -1.018000      88.91
 H      -4.494780    -0.862103    -1.080919      26.24
 O      -3.148476    -2.094796    -2.102417     263.80
 H      -3.546943    -3.022617    -1.818033      20.04
 C      -3.675123    -1.998653     0.296061      95.82
 H      -2.690652    -2.272463     0.623932      25.72
 O      -4.312724    -1.100574     1.330866     302.00
 H      -4.148149    -1.228843     2.234761      27.61
 C      -4.708772    -3.180135     0.342181      81.11
 O      -4.321617    -4.533533    -0.513690     237.46
 H      -3.516940    -4.982190    -0.038172      24.57
 H      -5.499476    -2.477810    -0.245049      25.93
 H      -5.265018    -3.499611     1.273364      27.50
55
name = lig-etoh-frame_312
 C       2.661634     1.762175    -2.117647      56.62
 H       2.295359     2.685477    -2.601782      22.64
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 C       3.481568     1.142738     0.192597      55.39
 H       3.871241     1.328796     1.183911      19.50
 C       4.028919    -0.027307    -0.412809      19.91
 O       4.777803    -0.809641     0.519204     230.88
 C       4.996641    -0.215110     1.814842     112.74
 H       4.029707    -0.027759     2.240729      26.17
 H       5.530100     0.754278     1.816905      27.25
 H       5.653775    -0.785868     2.509162      27.09
 C       4.101456    -0.154703    -1.772259      20.23
 O       4.822860    -1.194746    -2.458699     226.26
 H       4.742529    -1.942760    -1.750915      22.29
 C       3.315195     0.696885    -2.691905      41.72
 H       3.225472     0.260928    -3.625841      21.60
 C       2.807754     2.106996    -0.702934      39.45
 C       2.385375     3.489270    -0.231368     106.17
 H       3.083465     4.396137    -0.664598      20.51
 O       2.791176     3.710101     1.268212     277.29
 H       3.782069     3.917438     1.113070      26.51
 C       0.861441     3.532856    -0.210953      80.43
 H       0.451088     3.219686    -1.093061      22.90
 C       0.315689     4.919485     0.053067     114.18
 O       0.821580     5.885335    -0.833603     279.54
 H       0.630914     5.773812    -1.757280      29.78
 H       0.476963     5.067939     1.155969      24.54
 H      -0.852701     4.864405     0.117479      23.83
 C      -1.098524    -0.452512    -0.793381      39.52
 H      -0.789442    -1.514352    -0.855068      19.52
 C      -2.952697     1.049490    -0.248417      73.03
 H      -3.846563     1.526777    -0.774985      19.54
 C      -2.151963     1.987713     0.378250      -3.81
 O      -2.543483     3.241733     1.064242     174.82
 C      -3.967641     3.282479     1.075969     105.63
 H      -4.251147     3.452385    -0.131906      23.79
 H      -4.487853     2.455275     1.614204      26.26
 H      -4.227245     4.245920     1.628857      25.54
 C      -0.733024     1.810395     0.195912       2.88
 O       0.191928     2.648563     0.817179     183.07
 C      -0.210016     0.547769    -0.309411      26.32
 H       0.927170     0.335246    -0.609558      18.39
 C      -2.367689    -0.077749    -0.983908      28.81
 C      -3.531016    -1.148617    -1.083375      67.14
 H      -4.646788    -0.836079    -1.355172      23.49
 O      -3.119591    -2.088932    -2.022053     259.13
 H      -3.505743    -2.914294    -1.841340      24.58
 C      -3.699503    -2.013224     0.336799      72.20
 H      -2.714243    -2.443432     0.708436      22.71
 O      -4.335788    -1.096022     1.309550     242.38
 H      -4.022348    -1.322342     2.361959      21.84
 C      -4.706658    -3.177816     0.304771      88.12
 O      -4.260688    -4.598449    -0.473454     254.21
 H      -3.501715    -4.931360     0.032929      26.94
 H      -5.530291    -2.822481    -0.367836      26.72
 H      -5.055682    -3.503504     1.309149      27.47
55
name = lig-etoh-frame_313
 C       2.601259     1.768212    -2.110602      63.03
 H       2.539082     2.619348    -2.832223      23.06
 C       3.539531     1.199668     0.155041      51.29
 H       3.562656     1.399011     1.238385      17.48
 C       4.044710    -0.042926    -0.362971      13.63
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 O       4.838719    -0.828562     0.489733     202.02
 C       4.999290    -0.197247     1.823768     102.41
 H       3.917524    -0.240400     2.335861      24.46
 H       5.433343     0.829189     1.887698      25.56
 H       5.575135    -1.028050     2.261290      26.49
 C       4.105157    -0.129646    -1.747840      12.75
 O       4.833959    -1.204683    -2.438090     190.74
 H       4.814189    -1.964795    -1.709216      21.85
 C       3.353551     0.678117    -2.694328      33.98
 H       3.270998     0.094996    -3.693070      20.24
 C       2.765972     2.005736    -0.667733      59.87
 C       2.466096     3.443761    -0.251903      97.70
 H       2.896283     4.199760    -0.914729      22.59
 O       2.782563     3.708945     1.253448     260.06
 H       3.850686     3.845680     1.099125      25.44
 C       0.862741     3.579378    -0.238994      46.02
 H       0.330814     3.360064    -1.290424      19.50
 C       0.316274     4.972375     0.027876     118.09
 O       0.833154     5.944601    -0.780249     239.84
 H       0.544720     5.494325    -1.797166      23.51
 H       0.322392     5.100792     1.141399      24.22
 H      -0.759121     4.930861     0.125741      24.46
 C      -1.084294    -0.456971    -0.841837      23.13
 H      -0.520477    -1.419250    -1.000842      19.59
 C      -2.989986     1.093158    -0.270227      66.05
 H      -3.876295     1.540286    -0.707336      20.89
 C      -2.158326     2.006629     0.407997       1.28
 O      -2.518043     3.283872     1.101667     204.33
 C      -3.906207     3.337288     1.064201     128.91
 H      -4.419627     3.204723     0.130945      27.52
 H      -4.369776     2.406372     1.454400      26.46
 H      -4.318850     4.316088     1.367974      26.48
 C      -0.795616     1.832810     0.181179       4.46
 O       0.217818     2.603654     0.726474     178.40
 C      -0.203320     0.556169    -0.285433      10.77
 H       0.856937     0.329800    -0.498342      18.57
 C      -2.389730    -0.026841    -0.998901      25.50
 C      -3.537430    -1.016357    -1.115481      68.00
 H      -4.428072    -0.624536    -1.505468      25.71
 O      -3.072041    -2.106941    -1.984692     205.58
 H      -3.528419    -3.008824    -1.855101      21.08
 C      -3.726523    -2.007902     0.400900      49.01
 H      -2.747517    -2.424469     0.723846      22.04
 O      -4.344827    -1.096454     1.305621     311.04
 H      -3.816833    -1.370702     2.025808      26.85
 C      -4.694479    -3.222702     0.212620      86.04
 O      -4.217564    -4.600467    -0.429800     244.15
 H      -3.461435    -4.950908     0.272343      22.56
 H      -5.734662    -3.377933    -0.379233      23.28
 H      -4.825723    -3.454915     1.278208      26.93
55
name = lig-etoh-frame_314
 C       2.609095     1.770784    -2.110340      57.78
 H       2.394776     2.475044    -2.917882      22.00
 C       3.566632     1.223358     0.113739      81.27
 H       3.190767     1.590699     1.163277      17.34
 C       4.086553     0.000354    -0.285174      11.87
 O       4.898009    -0.833098     0.453654     192.84
 C       4.980550    -0.240876     1.847433     112.38
 H       4.099910    -0.341165     2.379575      28.73
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 H       5.386398     0.764576     1.849258      26.26
 H       5.609781    -1.094338     2.192091      26.78
 C       4.108662    -0.163977    -1.803367      18.75
 O       4.821199    -1.197091    -2.379486     223.23
 H       5.099722    -1.976635    -1.953316      24.07
 C       3.378135     0.630158    -2.635861      37.18
 H       3.342164     0.382091    -3.698063      23.03
 C       2.753131     1.950280    -0.698615      91.45
 C       2.457785     3.375962    -0.201067      96.99
 H       2.801084     4.105525    -1.114550      21.18
 O       2.799935     3.703912     1.185404     311.35
 H       3.724388     3.841791     1.393290      31.72
 C       0.837041     3.615878    -0.303806      59.27
 H       0.605094     3.373185    -1.289426      21.56
 C       0.277990     4.985902     0.097008     100.85
 O       0.842895     6.006959    -0.780183     208.32
 H       0.668202     5.677979    -1.586960      34.73
 H       0.665439     5.391630     1.095487      23.29
 H      -0.863899     4.920050    -0.232891      22.35
 C      -1.008346    -0.410916    -0.860798      45.73
 H      -0.620219    -1.304744    -1.245816      22.71
 C      -2.996981     1.169103    -0.332312      55.23
 H      -4.103782     1.342000    -0.482026      21.44
 C      -2.136277     2.073898     0.437748       4.67
 O      -2.474943     3.274920     1.102959     192.28
 C      -3.911638     3.380681     1.057024     104.35
 H      -4.446722     3.149076    -0.047997      23.93
 H      -4.256496     2.505256     1.678384      25.44
 H      -4.354429     4.424712     1.365735      24.65
 C      -0.766387     1.778288     0.184472      15.05
 O       0.259596     2.601904     0.639483     169.00
 C      -0.264957     0.564661    -0.290753      42.83
 H       0.863798     0.506902    -0.193243      18.24
 C      -2.505793     0.000159    -0.949332      -6.88
 C      -3.506065    -0.999680    -1.127974      65.51
 H      -4.420587    -0.357990    -1.544759      22.65
 O      -3.014152    -2.129569    -1.982582     195.47
 H      -3.581430    -2.943170    -1.752553      22.64
 C      -3.790389    -1.948976     0.359934      43.19
 H      -2.768973    -2.277418     0.668858      22.42
 O      -4.337800    -1.110499     1.314789     298.28
 H      -3.715736    -1.181555     2.150311      24.90
 C      -4.697874    -3.350274     0.117958      98.52
 O      -4.160632    -4.561332    -0.371048     346.07
 H      -3.579068    -5.018415     0.230968      28.50
 H      -5.698686    -3.329087    -0.198260      26.21
 H      -4.797123    -3.475453     1.256934      25.47
55
name = lig-etoh-frame_315
 C       2.679760     1.726426    -2.123151      48.43
 H       2.025439     2.381110    -2.771385      17.68
 C       3.542325     1.217405     0.130099      75.88
 H       3.327695     1.525556     1.083807      18.98
 C       4.153362     0.055673    -0.304922      21.42
 O       4.940253    -0.813066     0.436441     205.77
 C       5.004669    -0.356254     1.850111     104.61
 H       3.959095    -0.372614     2.480661      24.77
 H       5.413269     0.693544     1.812238      25.69
 H       5.794777    -0.900971     2.398573      27.56
 C       4.122765    -0.248556    -1.771838      25.67
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 O       4.810800    -1.187020    -2.347795     204.89
 H       5.388373    -1.991223    -1.982211      19.70
 C       3.357592     0.623774    -2.581249      66.92
 H       3.447183     0.664819    -3.687649      29.17
 C       2.742001     1.986505    -0.798193      78.19
 C       2.378373     3.343211    -0.161316     114.91
 H       2.878986     4.002121    -0.904991      24.83
 O       2.799752     3.695858     1.105505     294.62
 H       3.802564     3.854936     1.444138      29.37
 C       0.851364     3.624224    -0.324232      60.17
 H       0.726406     3.329271    -1.449048      19.60
 C       0.245478     5.010941     0.148913     106.57
 O       0.854533     6.075983    -0.774600     112.25
 H       0.755296     5.866112    -1.873009      26.43
 H       0.646644     5.394809     1.022023      25.67
 H      -0.768520     4.966040    -0.175488      24.70
 C      -1.043017    -0.334081    -0.888717      64.41
 H      -0.841131    -1.297563    -1.450429      22.06
 C      -3.004558     1.271725    -0.385783      56.28
 H      -4.079569     1.074712    -0.062968      22.08
 C      -2.094276     2.124139     0.412043       1.38
 O      -2.439924     3.252497     1.075954     173.76
 C      -3.965480     3.410494     1.052081     112.50
 H      -4.159693     3.285931     0.005344      25.95
 H      -4.325336     2.807306     1.896608      26.26
 H      -4.172589     4.357455     1.442674      27.60
 C      -0.728654     1.750527     0.225306      22.40
 O       0.303222     2.624837     0.567276     169.89
 C      -0.280842     0.573225    -0.303213      48.34
 H       0.795571     0.619078     0.138112      15.71
 C      -2.525942     0.011393    -0.856917     -24.19
 C      -3.514195    -1.071219    -1.138049      89.92
 H      -4.390000    -0.603555    -1.474285      24.74
 O      -2.966773    -2.134605    -1.992439     264.68
 H      -3.519064    -2.820688    -1.722749      26.67
 C      -3.848596    -1.877374     0.234371      63.68
 H      -2.787144    -2.167568     0.492197      22.20
 O      -4.332700    -1.126905     1.351259     331.11
 H      -3.840960    -0.894917     2.238090      25.39
 C      -4.693363    -3.453278     0.124831      80.68
 O      -4.113908    -4.516698    -0.367045     324.55
 H      -3.482204    -5.061739     0.329723      21.02
 H      -5.786517    -2.972546    -0.224705      24.44
 H      -4.910389    -3.567407     1.169369      26.55
55
name = lig-etoh-frame_316
 C       2.714757     1.707152    -2.145500      37.52
 H       1.867011     2.162691    -2.628990      19.56
 C       3.474279     1.206937     0.116342      52.50
 H       3.701319     1.421218     1.298996      17.95
 C       4.228840     0.094067    -0.386981      25.84
 O       4.977807    -0.793307     0.454076     266.31
 C       5.043702    -0.461390     1.857671     126.90
 H       4.128544    -0.470278     2.283071      28.72
 H       5.310371     0.593354     1.855346      27.01
 H       5.866855    -0.832448     2.505315      26.93
 C       4.107110    -0.281823    -1.666424      32.60
 O       4.836572    -1.226592    -2.368843     215.80
 H       5.394743    -1.774969    -1.717950      23.87
 C       3.355860     0.597343    -2.575618      74.87
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 H       3.603309     0.638351    -3.685092      27.53
 C       2.768344     2.048963    -0.800250      45.72
 C       2.300796     3.353304    -0.183748     119.02
 H       2.978884     4.176972    -0.833163      20.81
 O       2.793835     3.687625     1.089066     287.66
 H       3.764953     3.758915     0.876067      27.69
 C       0.880775     3.620471    -0.328453      84.79
 H       0.576058     3.456958    -1.354158      22.23
 C       0.271281     5.037229     0.089880      90.58
 O       0.857331     6.139100    -0.781146     174.32
 H       0.739824     5.902633    -1.773531      29.43
 H       0.437830     5.254671     1.285231      23.02
 H      -0.914120     5.037645     0.191160      22.96
 C      -1.202179    -0.288379    -0.949649      73.84
 H      -0.940005    -1.223127    -1.366301      24.15
 C      -3.009636     1.329655    -0.375409      66.18
 H      -3.903649     1.151338     0.183984      22.23
 C      -2.055326     2.130357     0.320153       0.55
 O      -2.431969     3.240028     1.050855     136.25
 C      -3.963262     3.448478     1.084279      91.90
 H      -4.260098     3.338128    -0.021486      24.41
 H      -4.585272     2.861546     1.883356      24.83
 H      -3.928791     4.614246     1.458744      23.75
 C      -0.715686     1.800430     0.278096      18.21
 O       0.335183     2.646212     0.538766     212.76
 C      -0.219875     0.593082    -0.274081      17.83
 H       0.784846     0.359074    -0.015352      18.26
 C      -2.478256     0.026558    -0.775815      -7.51
 C      -3.538247    -1.162667    -1.122413      88.21
 H      -4.585794    -0.892238    -1.632430      21.89
 O      -2.925736    -2.118502    -2.009200     239.88
 H      -3.421044    -3.014483    -1.819293      20.70
 C      -3.842960    -1.848053     0.143609      81.09
 H      -2.831305    -2.197454     0.344600      21.74
 O      -4.369255    -1.123314     1.372750     336.29
 H      -3.746256    -1.029938     2.055947      28.45
 C      -4.747443    -3.394756     0.206439      80.54
 O      -4.054846    -4.518344    -0.422784     331.73
 H      -3.440884    -4.837801     0.272014      25.48
 H      -5.525868    -3.145601    -0.433157      25.88
 H      -5.046283    -3.624648     1.303242      25.83
55
name = lig-etoh-frame_317
 C       2.693052     1.713158    -2.139741      40.19
 H       1.915198     2.113666    -2.837982      21.53
 C       3.443756     1.188828     0.115270      81.55
 H       3.800513     1.422054     1.003468      25.30
 C       4.287904     0.129607    -0.378857      35.77
 O       5.023860    -0.788100     0.468039     228.69
 C       5.109162    -0.504513     1.853102     106.15
 H       3.979101    -0.766617     2.311258      23.08
 H       5.221724     0.611881     2.025289      24.42
 H       5.875337    -1.124960     2.358395      25.69
 C       4.082481    -0.284702    -1.685336      21.06
 O       4.867444    -1.267225    -2.373476     227.66
 H       5.289384    -1.660358    -1.641341      26.43
 C       3.404405     0.533455    -2.593195      34.75
 H       3.599265     0.278228    -3.614349      22.25
 C       2.822355     2.093005    -0.713138      55.19
 C       2.298495     3.432192    -0.276976     109.27
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 H       2.704768     4.253211    -0.870329      23.60
 O       2.797860     3.669533     1.096469     317.81
 H       3.688608     3.715504     0.729095      26.97
 C       0.837081     3.654106    -0.333399      84.13
 H       0.385633     3.476830    -1.341837      21.76
 C       0.305362     5.073072     0.042840     120.71
 O       0.836402     6.174971    -0.762959     218.46
 H       0.635758     5.812131    -1.657109      31.82
 H       0.511872     5.135345     1.048086      26.30
 H      -0.754152     5.044217     0.237320      25.43
 C      -1.256116    -0.233003    -0.968511      41.64
 H      -0.936515    -1.258982    -1.247212      22.02
 C      -2.985059     1.316448    -0.310210      61.34
 H      -3.994800     1.424622     0.252113      20.39
 C      -2.058966     2.148120     0.217928      10.72
 O      -2.456845     3.227183     1.030836     182.25
 C      -3.914243     3.534543     1.124429     126.55
 H      -4.569937     3.437356     0.162817      26.15
 H      -4.558074     2.865515     1.655741      27.57
 H      -3.934303     4.486755     1.345280      28.65
 C      -0.642734     1.836464     0.277304      16.99
 O       0.356053     2.670829     0.581836     219.84
 C      -0.215934     0.588338    -0.258795      12.30
 H       0.845688     0.027418    -0.443146      17.60
 C      -2.562050     0.048782    -0.746785      10.89
 C      -3.603086    -1.201668    -1.137365      89.04
 H      -4.438106    -0.959579    -1.708443      23.31
 O      -2.888144    -2.119201    -2.030281     255.84
 H      -3.102613    -3.097822    -2.006974      20.21
 C      -3.830804    -1.911761     0.177108      79.23
 H      -2.799804    -2.354081     0.454744      19.15
 O      -4.413209    -1.113258     1.347247     293.44
 H      -3.540690    -1.338142     1.916610      21.47
 C      -4.779067    -3.272722     0.271187      73.01
 O      -4.014241    -4.494740    -0.495365     266.97
 H      -3.282849    -4.827012     0.170521      22.67
 H      -5.565810    -3.437862    -0.658976      22.12
 H      -5.099793    -3.530198     1.233647      26.89
55
name = lig-etoh-frame_318
 C       2.675053     1.687289    -2.119325      58.21
 H       2.225523     2.248401    -2.962198      23.90
 C       3.485372     1.154396     0.113443      57.78
 H       3.743501     1.670117     1.198858      19.31
 C       4.307307     0.131113    -0.324574      16.39
 O       5.073725    -0.773114     0.450738     241.65
 C       5.115457    -0.534779     1.877134     126.12
 H       4.309940    -0.971408     2.310115      28.50
 H       5.289277     0.461188     2.259328      26.22
 H       5.849693    -1.340458     2.092380      25.49
 C       4.112214    -0.296402    -1.774500      20.22
 O       4.871192    -1.270161    -2.352793     184.27
 H       5.366036    -1.923121    -1.631321      21.07
 C       3.422723     0.515503    -2.602010      48.68
 H       3.349052    -0.087995    -3.620455      20.27
 C       2.845232     2.119160    -0.717677      43.79
 C       2.316433     3.528176    -0.352338      85.73
 H       2.656206     4.439169    -1.165405      20.81
 O       2.793585     3.656429     1.083864     260.87
 H       3.897462     3.806664     1.196119      24.64
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 C       0.745873     3.695159    -0.363741      66.44
 H       0.314227     3.304698    -1.348646      21.63
 C       0.350716     5.095165     0.034654      99.47
 O       0.797754     6.179088    -0.742639     128.06
 H       0.511573     5.815547    -1.793082      25.49
 H       0.966648     5.279656     1.064021      22.11
 H      -0.816379     5.058751    -0.092621      22.50
 C      -1.219246    -0.183050    -0.921769      25.29
 H      -0.972875    -1.228321    -1.192581      21.43
 C      -3.013108     1.260952    -0.207670      50.05
 H      -4.001322     1.579307    -0.070447      22.34
 C      -2.030044     2.201470     0.165524       5.46
 O      -2.499890     3.223474     1.002280     192.17
 C      -3.867441     3.596290     1.122647     104.13
 H      -4.510013     3.614857     0.186916      25.77
 H      -4.362849     2.777061     1.834221      24.07
 H      -4.023898     4.758814     1.539512      23.47
 C      -0.564750     1.821591     0.212241       4.41
 O       0.374213     2.719115     0.685152     201.34
 C      -0.260150     0.536080    -0.310706      54.54
 H       0.654106     0.259018    -0.601065      21.28
 C      -2.729252     0.027750    -0.783461      -0.03
 C      -3.629374    -1.224023    -1.148019      69.37
 H      -4.556867    -0.776852    -1.735183      21.71
 O      -2.831430    -2.118119    -2.067783     247.93
 H      -3.005138    -3.036375    -1.925142      21.84
 C      -3.866233    -2.044410     0.274225      92.07
 H      -2.904011    -2.372847     0.599820      21.89
 O      -4.406846    -1.111750     1.293449     294.80
 H      -3.824058    -1.430612     2.099992      23.19
 C      -4.776579    -3.180750     0.200542      89.11
 O      -3.977364    -4.438511    -0.546873     246.18
 H      -3.285238    -4.924763     0.014060      25.29
 H      -5.653759    -3.274768    -0.307282      27.11
 H      -5.138302    -3.451017     1.274917      26.60
55
name = lig-etoh-frame_319
 C       2.700769     1.646630    -2.105631      81.63
 H       2.487689     2.442526    -2.843657      26.81
 C       3.567829     1.190491     0.170474      40.40
 H       3.483009     1.578924     1.120087      22.54
 C       4.293040     0.081275    -0.331283      10.80
 O       5.113904    -0.729850     0.416364     216.60
 C       5.145949    -0.613136     1.897323     108.84
 H       4.207869    -1.142201     2.469403      24.60
 H       5.477538     0.346449     2.399053      25.78
 H       6.013719    -1.290914     2.038038      25.87
 C       4.200707    -0.292197    -1.768240      23.42
 O       4.876469    -1.275431    -2.321517     257.37
 H       5.242247    -2.087355    -1.946954      23.04
 C       3.374287     0.509431    -2.635293      69.54
 H       3.022396     0.066666    -3.501902      22.79
 C       2.842676     2.121284    -0.831966      52.44
 C       2.365515     3.610811    -0.403413      90.34
 H       2.748930     4.295115    -1.147916      24.64
 O       2.801043     3.675612     1.063812     309.68
 H       3.624130     3.880172     1.365076      32.67
 C       0.722235     3.691944    -0.387805      73.72
 H       0.331066     3.298374    -1.294888      24.36
 C       0.371127     5.108848     0.079478     123.50
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 O       0.756907     6.169520    -0.790326     213.05
 H       0.565187     6.105696    -1.634667      35.72
 H       0.871589     5.347281     0.915058      27.03
 H      -0.708502     5.164837    -0.014283      25.82
 C      -1.302007    -0.214261    -0.866371      32.82
 H      -0.964433    -1.135312    -1.272518      21.22
 C      -3.068147     1.199447    -0.131948      41.59
 H      -4.124440     1.647506    -0.376412      19.19
 C      -1.975142     2.220999     0.165672      -1.88
 O      -2.509654     3.254088     0.965612     185.66
 C      -3.856989     3.656323     1.147328     118.39
 H      -4.314967     3.762693     0.075085      25.14
 H      -4.182738     2.998749     1.888264      26.90
 H      -3.884161     4.496352     1.720588      27.97
 C      -0.568560     1.823650     0.145746       1.29
 O       0.372767     2.771010     0.790503     171.79
 C      -0.291214     0.551150    -0.371345      50.30
 H       0.896143     0.478914    -0.597717      17.98
 C      -2.792327    -0.025594    -0.842345       1.47
 C      -3.626752    -1.235022    -1.144676      72.33
 H      -4.577987    -0.894350    -1.500684      26.69
 O      -2.787297    -2.095211    -2.102179     210.57
 H      -3.098570    -3.012642    -1.678759      18.52
 C      -3.907454    -2.099015     0.338769      74.76
 H      -2.854360    -2.422311     0.702930      22.49
 O      -4.386195    -1.124375     1.248726     316.62
 H      -4.233534    -1.276288     2.234457      26.59
 C      -4.765412    -3.210796     0.138953      83.28
 O      -3.965224    -4.351213    -0.597727     277.80
 H      -3.459711    -4.837979     0.105278      26.81
 H      -5.899290    -2.867965    -0.258369      25.78
 H      -4.938444    -3.482511     1.150205      29.00
55
name = lig-etoh-frame_320
 C       2.753439     1.645536    -2.141804      45.90
 H       2.472658     2.497034    -2.787255      21.60
 C       3.614592     1.267971     0.151434      76.81
 H       3.419841     1.429058     1.311572      17.89
 C       4.251090     0.055599    -0.357497      23.02
 O       5.153346    -0.686677     0.404246     221.95
 C       5.195461    -0.729334     1.920258     122.34
 H       4.326862    -1.021553     2.364909      30.53
 H       5.466017     0.258044     2.288306      28.29
 H       6.123382    -1.253524     2.165622      28.59
 C       4.247072    -0.238078    -1.719656      18.67
 O       4.887797    -1.292337    -2.335047     251.57
 H       5.141430    -2.233947    -1.975772      20.87
 C       3.321816     0.475644    -2.618914      54.12
 H       2.829866     0.245109    -3.674305      21.18
 C       2.872931     2.102550    -0.875708      55.67
 C       2.417512     3.588061    -0.404753      95.30
 H       3.001561     4.431819    -1.135025      22.26
 O       2.755178     3.713670     1.028013     227.03
 H       3.801328     4.058086     1.133776      27.06
 C       0.804725     3.685601    -0.342465      67.84
 H       0.274592     3.379980    -1.362831      21.01
 C       0.339253     5.110507     0.075685      99.50
 O       0.750507     6.186676    -0.834695     155.63
 H       0.436383     6.141100    -1.885967      25.56
 H       0.738382     5.359735     1.203076      23.98
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 H      -0.784494     5.194140     0.430578      24.07
 C      -1.429710    -0.310384    -0.835068      21.83
 H      -0.968608    -1.157619    -1.429444      18.82
 C      -3.115207     1.165027    -0.135571      56.91
 H      -4.055700     1.573830    -0.339071      21.18
 C      -2.007329     2.169415     0.206164      -0.17
 O      -2.446156     3.311549     0.925080     161.26
 C      -3.833553     3.686338     1.150617     101.54
 H      -4.339762     3.848215     0.226717      26.63
 H      -4.469603     2.896818     1.852248      23.94
 H      -3.650074     4.653101     1.877922      24.01
 C      -0.633642     1.881404     0.138966      -0.42
 O       0.339774     2.802236     0.837237     161.53
 C      -0.263199     0.635347    -0.432938      27.29
 H       0.748278     0.409899    -0.471191      19.55
 C      -2.745115    -0.041301    -0.847051      31.42
 C      -3.589785    -1.254298    -1.108147      74.70
 H      -4.709810    -1.144122    -1.444448      25.02
 O      -2.795756    -2.079462    -2.101008     232.94
 H      -3.011710    -2.956480    -1.728575      22.03
 C      -3.851327    -2.055674     0.367249      75.14
 H      -2.929134    -2.477263     0.667153      25.24
 O      -4.384610    -1.122863     1.204985     280.27
 H      -4.560294    -1.244395     2.268226      25.33
 C      -4.804954    -3.314849     0.084982      81.83
 O      -3.985420    -4.239098    -0.645008     329.81
 H      -3.668526    -4.683754     0.218526      24.18
 H      -5.578997    -2.781725    -0.314308      29.51
 H      -4.894994    -3.805931     1.125984      27.70
55
name = lig-etoh-frame_321
 C       2.808476     1.699725    -2.208847      27.32
 H       2.236880     2.310425    -2.935154      19.19
 C       3.619208     1.335970     0.087493      59.39
 H       3.567277     1.291564     1.180380      20.21
 C       4.214120     0.091070    -0.330224      16.34
 O       5.198717    -0.670286     0.413894     230.48
 C       5.276348    -0.792946     1.894436     110.49
 H       4.208798    -1.112413     2.343811      26.25
 H       5.341959     0.299020     2.179315      25.88
 H       6.116976    -1.459173     2.256630      26.82
 C       4.228785    -0.211812    -1.736222       7.37
 O       4.895824    -1.299490    -2.372095     203.34
 H       5.065997    -2.128451    -1.737219      21.60
 C       3.272801     0.427504    -2.595355      53.80
 H       3.170202     0.214467    -3.614353      25.97
 C       2.946005     2.099304    -0.797233      43.59
 C       2.457411     3.512499    -0.391667     112.45
 H       2.962877     4.360595    -0.849699      24.55
 O       2.740377     3.779512     0.990499     299.87
 H       3.667414     3.991633     0.759089      28.44
 C       0.902229     3.707414    -0.285306      74.70
 H       0.428164     3.466676    -1.147286      24.60
 C       0.290515     5.127874     0.101716     110.84
 O       0.744446     6.206537    -0.884126     189.97
 H       0.267523     5.813117    -1.739967      27.59
 H       0.770263     5.330548     1.008612      26.97
 H      -0.734527     5.036109     0.479463      25.04
 C      -1.376610    -0.370467    -0.824434      16.01
 H      -1.116513    -1.218987    -1.379195      18.66
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 C      -3.097097     1.172424    -0.184093      68.42
 H      -4.195703     1.513744    -0.115106      21.31
 C      -2.150059     2.085970     0.274357       9.54
 O      -2.362414     3.367322     0.879390     171.92
 C      -3.800418     3.693318     1.201389     121.16
 H      -4.506174     4.079117     0.296886      25.78
 H      -4.460332     2.979686     1.524059      27.80
 H      -3.629532     4.560865     1.800384      26.71
 C      -0.685416     1.931770     0.173917      -1.66
 O       0.280579     2.811025     0.813332     174.41
 C      -0.327826     0.708245    -0.485976      18.34
 H       0.732703     0.214958    -0.442827      17.88
 C      -2.721751    -0.025789    -0.794704      31.68
 C      -3.571030    -1.296852    -1.056608      87.12
 H      -4.557730    -1.252697    -1.494649      24.78
 O      -2.840217    -2.068830    -2.077101     247.04
 H      -2.891655    -3.028710    -1.921490      22.60
 C      -3.777537    -2.033807     0.354341      71.83
 H      -2.772387    -2.505695     0.732361      23.80
 O      -4.418998    -1.078765     1.181316     293.60
 H      -4.522790    -1.470979     2.005397      30.28
 C      -4.795252    -3.369562     0.095159      82.57
 O      -4.014416    -4.150400    -0.693377     326.74
 H      -3.546111    -4.767875    -0.062923      26.25
 H      -5.702675    -2.975579    -0.610566      25.46
 H      -5.215345    -3.961179     0.930962      27.21
55
name = lig-etoh-frame_322
 C       2.849082     1.760108    -2.239489      33.81
 H       2.062392     2.080046    -2.954460      19.80
 C       3.650923     1.310268     0.059567      41.19
 H       3.689241     1.558137     1.142255      18.52
 C       4.226576     0.126414    -0.316571       7.96
 O       5.240413    -0.674888     0.416621     250.95
 C       5.298756    -0.801814     1.855269     127.44
 H       4.410823    -1.247132     2.212314      29.16
 H       5.402267     0.187355     2.309269      27.35
 H       6.012407    -1.539572     2.148222      28.07
 C       4.180138    -0.243913    -1.765883       4.54
 O       4.878620    -1.274020    -2.385930     220.38
 H       5.135625    -1.822606    -1.693895      25.46
 C       3.260180     0.421984    -2.564301      64.64
 H       3.520539    -0.003989    -3.638991      24.79
 C       2.986475     2.154458    -0.793315      44.25
 C       2.425883     3.424565    -0.328255     111.21
 H       2.891002     4.354865    -1.045798      20.53
 O       2.766207     3.848385     0.967690     296.01
 H       3.767370     3.957232     1.012097      29.29
 C       0.951746     3.742890    -0.236014      50.47
 H       0.471798     3.362626    -1.281137      20.55
 C       0.312467     5.142091     0.125847      98.15
 O       0.696270     6.176337    -0.920324     194.22
 H       0.344897     5.734395    -1.668274      32.06
 H       0.994367     5.491321     1.006682      23.93
 H      -0.836214     4.949333     0.144331      22.51
 C      -1.249342    -0.325968    -0.818275      33.35
 H      -1.066305    -1.378056    -1.216314      19.03
 C      -3.119467     1.216006    -0.237159      63.06
 H      -4.144775     1.265459     0.137644      22.19
 C      -2.228401     2.063524     0.359866       3.15
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 O      -2.336242     3.400325     0.830544     184.72
 C      -3.757133     3.734083     1.199801     110.78
 H      -4.251069     4.221452     0.403192      27.76
 H      -4.372890     2.715372     1.548653      24.69
 H      -3.743962     4.563660     2.029859      25.39
 C      -0.744012     1.917678     0.202339      -3.43
 O       0.209087     2.803536     0.748029     172.48
 C      -0.418029     0.720753    -0.512283      45.08
 H       0.624625     0.338954    -0.496440      17.77
 C      -2.700028    -0.052031    -0.727814      -2.43
 C      -3.551223    -1.354267    -1.000433      82.46
 H      -4.553153    -1.067243    -1.495729      22.14
 O      -2.882049    -2.061580    -2.056558     242.98
 H      -2.947682    -3.108673    -2.016135      19.15
 C      -3.742964    -2.059522     0.327863      95.96
 H      -2.824395    -2.323917     0.784640      25.10
 O      -4.452207    -1.028164     1.158176     257.35
 H      -4.438517    -1.650232     1.968224      26.62
 C      -4.810428    -3.326970     0.101985      94.36
 O      -4.005119    -4.138879    -0.770477     319.60
 H      -3.381085    -4.799601    -0.456792      29.72
 H      -5.605309    -3.286540    -0.587848      26.06
 H      -5.465813    -3.877529     0.864940      25.62
55
name = lig-etoh-frame_323
 C       2.857180     1.774741    -2.223450      48.16
 H       2.065964     2.187734    -2.851101      18.25
 C       3.692177     1.269393     0.096980      27.92
 H       3.864949     1.952573     1.020444      18.84
 C       4.307259     0.096751    -0.353094       6.58
 O       5.269405    -0.676518     0.392335     247.15
 C       5.291863    -0.791438     1.811809     110.50
 H       4.334251    -1.347805     2.205044      25.09
 H       5.584680     0.056155     2.516295      24.89
 H       6.161128    -1.546701     1.939743      25.40
 C       4.121625    -0.287178    -1.730005      14.67
 O       4.840673    -1.220539    -2.382752     180.35
 H       5.453326    -1.765647    -1.672084      21.57
 C       3.300765     0.452123    -2.573181      73.14
 H       3.430075     0.018508    -3.541429      27.81
 C       2.992054     2.192292    -0.893161      79.56
 C       2.395775     3.447535    -0.268253     105.07
 H       2.542688     3.963556    -1.213697      26.28
 O       2.839076     3.920276     0.986712     302.78
 H       3.790513     3.868402     1.417645      27.72
 C       0.897621     3.721090    -0.257633      59.32
 H       0.622663     3.482775    -1.202395      21.40
 C       0.398709     5.153746     0.125303     107.99
 O       0.630316     6.122778    -0.931432     195.55
 H       0.510766     5.698086    -2.013777      24.10
 H       0.744758     5.645535     1.070401      24.34
 H      -0.669437     5.027581    -0.051255      22.24
 C      -1.233672    -0.275845    -0.833168      65.14
 H      -0.766438    -1.263049    -0.920512      20.58
 C      -3.181547     1.210894    -0.262893      45.79
 H      -4.187408     1.116439     0.157394      21.05
 C      -2.174226     2.124610     0.429671       0.42
 O      -2.376359     3.424538     0.799991     192.13
 C      -3.705002     3.765666     1.222748     115.41
 H      -4.080934     4.359702     0.252520      24.11
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 H      -4.073514     2.893738     1.498809      27.97
 H      -3.830246     4.248112     2.244575      25.46
 C      -0.834186     1.857365     0.205899      13.04
 O       0.136217     2.783947     0.676764     166.70
 C      -0.430237     0.737906    -0.492337      43.51
 H       0.681202     0.662904    -0.605207      15.75
 C      -2.623260    -0.113853    -0.666160     -17.62
 C      -3.540872    -1.362174    -0.978269      86.23
 H      -4.492726    -0.842545    -1.232977      23.55
 O      -2.904475    -2.072259    -2.054496     272.87
 H      -3.250141    -2.953369    -1.898308      19.74
 C      -3.812591    -2.086270     0.306165      99.46
 H      -2.828888    -2.302971     0.878115      21.12
 O      -4.475064    -1.013222     1.143158     254.80
 H      -4.425284    -1.451532     2.142039      25.70
 C      -4.793254    -3.280592     0.097649      76.61
 O      -3.982782    -4.176132    -0.878551     275.61
 H      -3.262024    -4.779772    -0.415034      24.72
 H      -5.667641    -3.005365    -0.651109      25.50
 H      -5.237678    -3.707131     1.033339      26.85
55
name = lig-etoh-frame_324
 C       2.824642     1.752036    -2.206351      39.51
 H       2.255729     2.482322    -2.838809      21.44
 C       3.721022     1.301642     0.093314      83.27
 H       4.079579     1.807372     0.921341      29.82
 C       4.400695     0.071640    -0.367580      17.88
 O       5.291136    -0.666102     0.342818     252.99
 C       5.298441    -0.819463     1.793579     118.89
 H       4.369273    -1.203003     2.208015      26.43
 H       5.630614     0.000404     2.436917      25.81
 H       6.136606    -1.448456     1.806393      25.94
 C       4.064988    -0.309101    -1.663385      36.43
 O       4.821711    -1.196375    -2.360092     213.17
 H       5.576847    -1.691843    -1.967786      23.34
 C       3.353612     0.514469    -2.584879      39.26
 H       3.116001     0.184049    -3.666600      19.07
 C       3.014453     2.152891    -0.910977      59.05
 C       2.370301     3.485725    -0.244443      86.26
 H       2.517211     4.216601    -1.285020      22.04
 O       2.905333     3.997283     1.041969     274.58
 H       3.851613     3.799749     1.174650      29.23
 C       0.816698     3.658091    -0.249387      59.83
 H       0.511944     3.581873    -1.416231      16.28
 C       0.457036     5.153622     0.067429     118.60
 O       0.591959     6.079433    -0.979254     292.95
 H       0.609647     5.700577    -1.775421      33.42
 H       0.528243     5.625401     1.121020      24.20
 H      -0.688419     5.045336     0.209646      23.09
 C      -1.251894    -0.275609    -0.845140      64.01
 H      -0.598830    -1.156637    -0.870883      20.22
 C      -3.180159     1.161002    -0.231499      33.20
 H      -4.309608     1.133923    -0.011139      20.19
 C      -2.171864     2.170946     0.430152      -0.54
 O      -2.411612     3.461588     0.795745     208.01
 C      -3.658467     3.806648     1.227135     119.66
 H      -4.150919     4.346423     0.498020      27.52
 H      -4.302093     2.716306     1.326671      23.36
 H      -3.655321     4.263958     2.227813      26.36
 C      -0.878406     1.832380     0.199839      20.76
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 O       0.071295     2.764503     0.615631     174.19
 C      -0.354398     0.778633    -0.445769      32.08
 H       0.744366     0.991740    -0.783163      14.77
 C      -2.576919    -0.148682    -0.606704      10.44
 C      -3.504606    -1.281200    -0.965971      69.98
 H      -4.525024    -0.808601    -1.164859      23.64
 O      -2.939545    -2.087817    -2.048689     233.25
 H      -3.488138    -2.940363    -1.892718      17.18
 C      -3.897634    -2.095325     0.333811     100.66
 H      -3.023651    -2.464703     0.814177      21.72
 O      -4.500498    -1.031046     1.149492     362.72
 H      -4.396827    -1.058266     2.037220      31.50
 C      -4.753473    -3.236498     0.045651      79.67
 O      -3.969449    -4.234622    -0.962782     301.48
 H      -3.421158    -4.552975    -0.226466      26.80
 H      -5.554405    -2.668956    -0.402802      28.22
 H      -4.858509    -3.673170     1.064817      28.07
55
name = lig-etoh-frame_325
 C       2.773828     1.744075    -2.197244      66.97
 H       2.563744     2.551357    -2.906759      26.52
 C       3.770624     1.328991     0.024868      45.16
 H       4.257435     1.587516     1.088564      20.99
 C       4.422604     0.124452    -0.348062      21.73
 O       5.324119    -0.661520     0.294122     255.88
 C       5.326977    -0.836211     1.767167     106.02
 H       4.327278    -1.137550     2.203754      26.02
 H       5.588893     0.179101     2.200584      24.47
 H       6.139698    -1.651469     1.939933      24.73
 C       4.041961    -0.315000    -1.644064      33.39
 O       4.806916    -1.205992    -2.367562     199.79
 H       5.497127    -1.691222    -1.966374      25.35
 C       3.376218     0.581622    -2.613094      48.16
 H       2.946128     0.305356    -3.599499      20.32
 C       3.039275     2.119226    -0.786986      39.77
 C       2.364450     3.536116    -0.290749      94.51
 H       2.670049     4.440884    -0.726983      21.38
 O       2.941781     4.053333     1.073576     235.92
 H       3.944809     3.908296     0.776771      25.96
 C       0.753871     3.603313    -0.265196      72.58
 H       0.378978     3.512484    -1.240188      21.97
 C       0.400190     5.125731     0.029200     106.27
 O       0.587950     6.072681    -1.003055     240.46
 H       0.551524     5.463114    -1.965907      23.19
 H       0.852691     5.531161     1.050647      23.39
 H      -0.635137     4.976531     0.415241      23.44
 C      -1.169414    -0.268172    -0.824538      29.01
 H      -0.737486    -1.297814    -1.157176      20.72
 C      -3.118640     1.113241    -0.142920      53.41
 H      -4.162714     1.266759    -0.252066      23.09
 C      -2.280887     2.151887     0.357167       5.15
 O      -2.407538     3.493808     0.790769     216.67
 C      -3.699976     3.779289     1.251688     122.56
 H      -4.382486     4.580865     0.631978      24.95
 H      -4.400708     3.088716     1.231332      27.53
 H      -3.427959     4.430788     2.214341      23.76
 C      -0.856272     1.871902     0.195361      14.12
 O       0.032018     2.773399     0.586539     203.39
 C      -0.280208     0.785934    -0.443554      43.88
 H       0.668616     0.917120    -0.812771      18.49
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 C      -2.591296    -0.130970    -0.557915      25.68
 C      -3.481802    -1.193195    -0.945445      69.81
 H      -4.472399    -0.859251    -1.350966      22.61
 O      -2.993334    -2.094344    -2.027786     219.75
 H      -3.495860    -3.004759    -2.073647      16.34
 C      -3.898544    -2.043997     0.374490      93.33
 H      -2.995535    -2.570076     0.854435      18.90
 O      -4.551953    -1.059712     1.138018     328.97
 H      -4.166446    -0.894284     2.127394      24.88
 C      -4.724176    -3.210476    -0.019457      74.16
 O      -3.992817    -4.268972    -0.990803     292.54
 H      -3.444381    -4.550272    -0.215001      24.82
 H      -5.762319    -2.790282    -0.285284      26.53
 H      -4.744331    -3.900040     0.900289      27.41
55
name = lig-etoh-frame_326
 C       2.762112     1.780966    -2.126196      70.34
 H       2.617795     2.499580    -2.950979      27.46
 C       3.885893     1.338258     0.045757      34.02
 H       4.030031     1.591541     1.026427      21.22
 C       4.384623     0.172144    -0.380319      24.82
 O       5.370114    -0.674337     0.262669     270.61
 C       5.368421    -0.831613     1.732680     118.89
 H       4.317095    -1.048974     2.100623      26.98
 H       5.613932     0.186126     2.031159      26.46
 H       5.946824    -1.617690     2.136305      27.17
 C       4.058248    -0.288169    -1.693082      26.58
 O       4.778874    -1.236979    -2.394479     171.17
 H       5.330704    -1.827606    -1.653616      21.42
 C       3.358749     0.617357    -2.616050      53.22
 H       3.147885     0.214443    -3.620414      19.17
 C       3.002746     2.169422    -0.693325      67.63
 C       2.368495     3.562056    -0.293097      97.74
 H       2.792135     4.563512    -0.761370      20.30
 O       2.958092     4.065752     1.077259     209.62
 H       3.935305     4.275937     0.799138      27.92
 C       0.744095     3.610720    -0.300361      63.41
 H       0.283429     3.293309    -1.361591      21.52
 C       0.319963     5.075167     0.052743      95.33
 O       0.599394     6.043744    -1.051109     216.10
 H       0.287687     5.629158    -1.923090      27.30
 H       1.237703     5.392040     0.795909      23.30
 H      -0.736193     5.057355     0.341262      24.75
 C      -1.092766    -0.280151    -0.786031      53.59
 H      -0.999655    -1.150578    -1.387874      20.93
 C      -3.073695     1.091528    -0.036619      75.90
 H      -4.117379     1.402431    -0.446376      20.63
 C      -2.305979     2.120887     0.261235       9.57
 O      -2.421507     3.488231     0.763294     181.84
 C      -3.772854     3.860132     1.286977     122.91
 H      -4.136542     4.634705     0.723238      28.72
 H      -4.626144     2.946856     1.445505      24.09
 H      -3.576415     4.299316     2.196676      28.36
 C      -0.854946     1.902208     0.170064       8.53
 O       0.028247     2.822700     0.620135     184.95
 C      -0.269359     0.755474    -0.464377      33.43
 H       0.903165     0.660523    -0.801737      16.18
 C      -2.533876    -0.086288    -0.545284      17.37
 C      -3.508274    -1.190913    -0.941998      75.70
 H      -4.410174    -0.752815    -1.409004      23.39
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 O      -3.028174    -2.080884    -2.013460     277.48
 H      -3.426283    -2.910665    -2.018488      22.29
 C      -3.824753    -1.974418     0.376806      88.42
 H      -2.943455    -2.330759     0.907049      23.69
 O      -4.624728    -1.085217     1.165223     338.82
 H      -3.899252    -1.005167     1.902603      25.68
 C      -4.735942    -3.242143    -0.067295     105.46
 O      -4.044093    -4.268899    -0.979766     285.27
 H      -3.327696    -4.804824    -0.453910      25.41
 H      -5.810185    -3.292536    -0.353189      26.38
 H      -4.919399    -3.948972     0.713807      25.89
55
name = lig-etoh-frame_327
 C       2.795957     1.841660    -2.027171      46.93
 H       2.328092     2.503063    -2.796609      19.28
 C       3.948299     1.407117     0.114401      67.29
 H       3.916241     1.775275     1.223811      13.55
 C       4.376983     0.132820    -0.448414      12.86
 O       5.411272    -0.699673     0.226173     238.08
 C       5.364913    -0.779790     1.682810     112.94
 H       4.319451    -0.925920     1.982676      28.25
 H       5.774191     0.151306     2.174875      27.50
 H       5.999647    -1.619989     2.153899      26.51
 C       4.092324    -0.218015    -1.796528      17.30
 O       4.752252    -1.292779    -2.387834     229.00
 H       4.969141    -1.877934    -1.670751      25.65
 C       3.323946     0.609704    -2.575256      41.04
 H       3.517840     0.240988    -3.666733      23.67
 C       2.950547     2.244703    -0.680955      91.52
 C       2.401745     3.597826    -0.253167      99.58
 H       2.623201     4.160367    -1.225957      25.04
 O       2.943367     4.061048     1.065680     276.12
 H       3.840059     4.410887     1.085501      32.74
 C       0.746490     3.657034    -0.378066      61.88
 H       0.519367     3.199861    -1.324016      22.24
 C       0.282672     5.040606     0.051145     104.70
 O       0.600865     6.008326    -1.085444     201.07
 H       0.143337     5.751734    -1.980913      26.40
 H       1.220590     5.246828     0.636961      26.92
 H      -0.763341     5.264949     0.373084      25.00
 C      -1.117156    -0.307712    -0.746210      65.51
 H      -0.956870    -1.078199    -1.630071      20.08
 C      -3.117614     1.069775     0.014432      63.98
 H      -4.076549     1.296645    -0.298313      21.53
 C      -2.176082     2.175160     0.215388       7.83
 O      -2.486777     3.447151     0.728209     153.20
 C      -3.849754     3.910781     1.321393     103.36
 H      -4.042489     4.756875     0.520023      23.67
 H      -4.404773     3.086355     1.530504      25.90
 H      -3.720679     4.209853     2.490418      24.84
 C      -0.839570     1.891678     0.119660      11.64
 O       0.043734     2.879669     0.699550     163.83
 C      -0.231440     0.736285    -0.485458      37.84
 H       0.741492     0.580456    -0.552678      18.60
 C      -2.438920    -0.073701    -0.566865       1.83
 C      -3.526988    -1.210719    -0.957225      76.41
 H      -4.449825    -0.577226    -1.236321      23.27
 O      -3.030953    -2.035217    -2.007670     249.95
 H      -3.462533    -3.007397    -1.780053      14.28
 C      -3.812647    -1.935556     0.310464      81.08
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 H      -2.863266    -2.135548     0.892166      22.15
 O      -4.672535    -1.119465     1.217712     338.63
 H      -4.072454    -0.983744     1.877870      30.79
 C      -4.735955    -3.349150    -0.079844      86.96
 O      -4.092546    -4.262113    -0.972401     288.24
 H      -3.434861    -4.844745    -0.627172      28.81
 H      -5.696661    -3.318245    -0.688943      24.64
 H      -5.016101    -3.838780     0.969303      24.10
55
name = lig-etoh-frame_328
 C       2.829268     1.888051    -1.974713      63.34
 H       2.039205     2.460416    -2.485351      17.83
 C       3.923957     1.488395     0.163424      21.59
 H       4.098122     1.749989     1.203346      15.62
 C       4.405266     0.119810    -0.457735       2.08
 O       5.433961    -0.720766     0.176284     205.20
 C       5.362944    -0.708987     1.645644     111.76
 H       4.254773    -0.788048     1.968654      26.05
 H       5.864318     0.079506     2.238497      27.46
 H       5.965546    -1.587323     1.841442      27.31
 C       4.159155    -0.166239    -1.862755      12.21
 O       4.705124    -1.342489    -2.378822     241.36
 H       4.832846    -2.058780    -1.720369      23.95
 C       3.293530     0.628336    -2.551005      75.57
 H       3.483642     0.570269    -3.586317      29.23
 C       2.968198     2.261532    -0.659987      54.92
 C       2.426533     3.618125    -0.235450      86.45
 H       2.566016     4.054790    -1.293745      24.07
 O       2.878273     4.051231     1.034427     238.94
 H       3.900444     4.353045     1.194885      27.51
 C       0.771577     3.688057    -0.387313      59.85
 H       0.630322     3.247836    -1.434089      18.21
 C       0.285535     5.056365    -0.038071      99.35
 O       0.601993     5.982201    -1.094788     259.67
 H       0.077407     5.744321    -2.070283      22.50
 H       0.996406     5.370433     0.956214      24.05
 H      -0.641195     5.199809     0.461458      24.89
 C      -1.127675    -0.344120    -0.769591      69.51
 H      -0.737739    -1.016049    -1.420088      21.35
 C      -3.083914     1.075882     0.018862      48.01
 H      -4.275898     1.123437     0.022622      18.43
 C      -2.117922     2.215517     0.216139       1.68
 O      -2.564776     3.417139     0.704326     168.32
 C      -3.855593     3.948915     1.344341     110.81
 H      -4.220437     4.637632     0.622271      26.84
 H      -4.611346     2.979462     1.344355      22.67
 H      -3.682560     4.321000     2.264769      27.94
 C      -0.728464     1.893982     0.084491      10.53
 O       0.067880     2.911018     0.763242     146.33
 C      -0.234912     0.733896    -0.471151      34.82
 H       0.973036     0.604998    -0.347516      13.93
 C      -2.476265    -0.084475    -0.584172      12.23
 C      -3.512990    -1.155409    -0.979030      86.39
 H      -4.447637    -0.636696    -1.157964      23.54
 O      -3.041779    -2.008041    -2.003704     301.85
 H      -3.269415    -2.903394    -1.732051      19.59
 C      -3.869258    -1.951801     0.260201      72.28
 H      -2.893068    -2.166992     0.746373      21.94
 O      -4.711749    -1.170661     1.247003     294.23
 H      -4.261748    -0.894861     2.208085      24.84
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 C      -4.746368    -3.444114    -0.038333      85.64
 O      -4.126904    -4.273139    -0.987274     307.84
 H      -3.479339    -4.836296    -0.469420      26.23
 H      -5.447623    -2.870310    -0.737956      26.11
 H      -4.981111    -3.657755     0.940565      27.61
55
name = lig-etoh-frame_329
 C       2.830392     1.890861    -1.961632      40.59
 H       1.948928     2.385298    -2.397869      17.45
 C       3.885094     1.484972     0.151185      38.15
 H       4.317329     1.707277     1.154772      17.92
 C       4.451232     0.188052    -0.430653      15.60
 O       5.420592    -0.706743     0.123389     238.80
 C       5.360531    -0.659723     1.604413     112.81
 H       4.364428    -0.702069     1.974561      27.94
 H       5.906786     0.188314     2.068318      26.75
 H       5.835287    -1.655865     1.745931      26.26
 C       4.243891    -0.165025    -1.829137       6.22
 O       4.645099    -1.373957    -2.391198     204.84
 H       4.831149    -2.201158    -1.727587      20.85
 C       3.271873     0.716887    -2.549057      71.76
 H       3.096811     0.855788    -3.729909      27.94
 C       3.052958     2.241396    -0.587379      49.47
 C       2.412486     3.606923    -0.259540     103.76
 H       2.784536     4.510729    -0.951046      23.21
 O       2.808068     4.059501     1.014051     266.89
 H       3.762033     4.039047     0.935790      29.76
 C       0.836707     3.694428    -0.319138      64.27
 H       0.485663     3.417993    -1.371465      19.28
 C       0.345843     5.117949    -0.106807     116.20
 O       0.596240     5.984540    -1.098464     348.10
 H       0.338536     5.606658    -1.930903      30.75
 H       0.520089     5.495062     0.878392      24.81
 H      -0.802459     4.905478     0.252112      21.98
 C      -1.105875    -0.321971    -0.806107      31.20
 H      -0.536512    -1.323986    -1.195599      17.90
 C      -2.999872     1.117401    -0.010520      49.56
 H      -3.951816     1.026085     0.442640      19.82
 C      -2.165389     2.176372     0.238616       1.15
 O      -2.625744     3.429053     0.693590     195.02
 C      -3.852892     3.880699     1.306519     120.31
 H      -4.406779     4.676468     0.645325      25.30
 H      -4.705521     3.225542     1.274287      25.03
 H      -3.533774     4.515989     2.288561      23.62
 C      -0.630224     1.957906     0.106089       3.74
 O       0.111615     2.912804     0.772457     184.53
 C      -0.205915     0.714400    -0.422637      41.25
 H       0.810740     0.619186    -0.339081      16.05
 C      -2.580359    -0.099791    -0.598017      17.64
 C      -3.514244    -1.080852    -0.977910      85.36
 H      -4.532590    -0.679827    -1.405292      22.17
 O      -3.042809    -1.979638    -2.017310     295.64
 H      -3.142656    -2.928119    -1.786700      19.58
 C      -3.922116    -2.015384     0.285118      76.05
 H      -2.957484    -2.341533     0.700129      21.61
 O      -4.747882    -1.226364     1.258443     332.39
 H      -4.386033    -1.158113     2.195788      26.86
 C      -4.751573    -3.383920    -0.035776      83.21
 O      -4.135299    -4.323869    -0.988433     304.02
 H      -3.553813    -4.813824    -0.297303      25.70
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 H      -5.512020    -2.734605    -0.411212      27.37
 H      -5.115944    -3.830360     1.030198      26.44
55
name = lig-etoh-frame_330
 C       2.795474     1.880730    -1.921653      33.05
 H       2.055633     2.411057    -2.521520      22.24
 C       3.915140     1.384205     0.154360      55.24
 H       4.432918     1.769241     1.102796      26.01
 C       4.501929     0.280176    -0.453220      43.09
 O       5.375361    -0.657319     0.095474     261.93
 C       5.387435    -0.644578     1.546402     102.33
 H       4.296447    -0.568991     2.005313      24.17
 H       5.984838     0.257105     1.810198      25.00
 H       5.752592    -1.619745     1.995998      25.04
 C       4.261338    -0.148662    -1.774323      15.09
 O       4.578724    -1.395511    -2.408733     251.18
 H       4.914567    -2.004599    -1.792793      25.52
 C       3.297142     0.804830    -2.584394      47.08
 H       2.818087     0.668324    -3.501863      20.66
 C       3.107085     2.259368    -0.575669      43.39
 C       2.395130     3.611390    -0.278818     113.72
 H       2.857479     4.566312    -0.767063      17.80
 O       2.748173     4.067617     1.024669     301.39
 H       3.725969     3.840303     0.912567      23.44
 C       0.917556     3.713053    -0.236805      61.68
 H       0.388816     3.447775    -1.168212      17.17
 C       0.311736     5.132985    -0.100485      98.86
 O       0.606341     6.042140    -1.104064     260.50
 H       0.679980     5.436363    -2.103546      22.51
 H       0.539795     5.723504     0.882820      21.03
 H      -0.729010     4.796815    -0.379590      19.63
 C      -1.103021    -0.292122    -0.838874      39.84
 H      -0.783316    -1.268727    -0.829605      22.65
 C      -2.936701     1.124469    -0.037768      57.20
 H      -3.815751     1.117391     0.703609      19.11
 C      -2.156622     2.154573     0.277679       5.93
 O      -2.658452     3.447116     0.678979     204.48
 C      -3.856512     3.848029     1.249056     137.04
 H      -4.229664     4.663882     0.636744      26.99
 H      -4.744906     3.098584     1.532251      24.53
 H      -3.618739     4.290359     2.188386      27.21
 C      -0.655930     2.017302     0.157193       2.59
 O       0.190327     2.907691     0.742400     199.68
 C      -0.201749     0.714797    -0.351864      18.63
 H       0.957381     0.463458    -0.421478      15.33
 C      -2.556695    -0.082789    -0.619226       8.12
 C      -3.610949    -1.103430    -0.981167      81.74
 H      -4.414856    -0.659166    -1.489882      23.66
 O      -3.026642    -1.944791    -2.047379     264.35
 H      -3.135336    -2.978140    -1.778072      15.90
 C      -3.951107    -2.086593     0.348215      84.60
 H      -2.964350    -2.441848     0.806655      20.27
 O      -4.779333    -1.297177     1.247854     337.99
 H      -4.353362    -1.532417     2.086706      26.60
 C      -4.779508    -3.254886    -0.011667      99.69
 O      -4.140639    -4.371648    -0.951311     283.19
 H      -3.634017    -4.867283    -0.323161      28.97
 H      -5.933225    -3.047237    -0.336505      25.90
 H      -5.045404    -3.938780     0.716162      27.53
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name = lig-etoh-frame_331
 C       2.749210     1.889404    -1.880250      77.27
 H       2.200140     2.579162    -2.560873      22.22
 C       3.970838     1.334819     0.185466      85.04
 H       4.353784     1.710083     1.068672      26.98
 C       4.568518     0.314840    -0.526427      16.31
 O       5.332193    -0.620436     0.099949     271.63
 C       5.401084    -0.621434     1.512528     112.93
 H       4.454093    -0.372666     1.884674      28.90
 H       6.063905     0.209720     1.773339      26.47
 H       5.822996    -1.459908     2.041370      26.30
 C       4.178747    -0.093808    -1.810636      16.09
 O       4.503451    -1.371975    -2.415640     209.63
 H       5.114011    -1.891385    -1.761512      22.54
 C       3.380620     0.811354    -2.576383      42.21
 H       2.752432     0.200874    -3.401749      21.41
 C       3.114676     2.291971    -0.626562      34.67
 C       2.417498     3.624037    -0.248545      92.36
 H       2.778105     4.332661    -1.153604      20.82
 O       2.723373     4.065525     1.077809     262.60
 H       3.741432     3.917140     1.340837      25.96
 C       0.950717     3.746964    -0.198526      69.74
 H       0.507077     3.344491    -1.209690      17.91
 C       0.235947     5.127392    -0.076916     104.15
 O       0.663785     6.113394    -1.150481     264.79
 H       0.697461     5.782316    -1.970499      32.82
 H       0.410566     5.723379     0.835452      23.17
 H      -0.728858     4.936691    -0.573883      21.10
 C      -1.141159    -0.228588    -0.821042      42.59
 H      -0.911253    -1.384068    -0.758498      20.53
 C      -2.950279     1.090359    -0.027327      47.50
 H      -3.901571     1.204017     0.498690      20.01
 C      -2.057179     2.215175     0.329297      15.84
 O      -2.637828     3.436677     0.647278     210.64
 C      -3.905372     3.808413     1.207971     121.71
 H      -4.210797     4.630653     0.525991      25.01
 H      -4.485381     2.955247     1.632780      24.37
 H      -3.670550     4.193920     2.348863      24.48
 C      -0.732942     2.012785     0.201005      16.49
 O       0.287658     2.900795     0.726252     195.93
 C      -0.206261     0.735697    -0.281560      25.71
 H       0.830461     0.425462    -0.441359      17.08
 C      -2.475949    -0.061300    -0.646246      12.23
 C      -3.669626    -1.194613    -0.968050      61.82
 H      -4.583451    -0.543109    -1.379640      22.08
 O      -3.008072    -1.931642    -2.073161     298.69
 H      -3.214738    -2.802954    -1.860508      21.19
 C      -3.972994    -2.105704     0.362942      93.49
 H      -3.069348    -2.403481     0.859806      19.82
 O      -4.792757    -1.370267     1.248928     286.21
 H      -4.427738    -1.859370     2.177006      22.61
 C      -4.875127    -3.211281    -0.021727     114.09
 O      -4.152865    -4.383603    -0.910187     264.25
 H      -3.651509    -4.971639    -0.258512      26.39
 H      -5.791209    -3.292864    -0.449905      28.14
 H      -4.889765    -3.978531     0.889458      25.71
55
name = lig-etoh-frame_332
 C       2.730417     1.902013    -1.913493      75.68
 H       2.256371     2.685777    -2.484213      21.11
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 C       3.984072     1.387847     0.158086      79.42
 H       4.297881     1.623174     1.300210      23.09
 C       4.621289     0.316936    -0.577518      10.29
 O       5.320451    -0.632485     0.101094     241.19
 C       5.431437    -0.549208     1.502517      96.25
 H       4.390989    -0.206911     1.946475      24.31
 H       6.176263     0.226909     1.877879      25.87
 H       5.897092    -1.561604     1.848472      23.84
 C       4.095460    -0.061716    -1.896065      32.55
 O       4.425286    -1.319150    -2.394686     199.10
 H       5.258193    -1.701435    -1.882608      22.56
 C       3.405944     0.756400    -2.562836      71.88
 H       3.011749     0.138903    -3.285299      24.69
 C       3.117464     2.290048    -0.639190      35.25
 C       2.490764     3.638002    -0.195759      71.34
 H       2.718634     4.231283    -1.257762      21.14
 O       2.735517     4.068831     1.165369     299.14
 H       3.591272     4.122548     1.480716      30.91
 C       0.910013     3.765570    -0.242261      69.27
 H       0.791976     3.399787    -1.259891      18.30
 C       0.176241     5.142531    -0.138126      93.92
 O       0.749247     6.209424    -1.142601     207.03
 H       0.517135     5.846086    -2.235475      21.67
 H       0.159376     5.598737     0.912090      23.60
 H      -0.951642     5.032388    -0.203078      22.39
 C      -1.123244    -0.204192    -0.756923      59.76
 H      -0.807951    -1.191952    -1.052545      22.96
 C      -2.957706     1.106995     0.008594      60.56
 H      -4.098119     1.176572     0.068751      19.21
 C      -2.060659     2.245111     0.370037      14.46
 O      -2.579862     3.440674     0.615022     203.18
 C      -3.915533     3.755006     1.226605     119.84
 H      -4.504182     4.445214     0.508569      25.47
 H      -4.516969     2.795953     1.349441      23.79
 H      -3.734319     4.281401     2.137882      27.53
 C      -0.688235     1.981653     0.244047      21.79
 O       0.362839     2.870224     0.742775     176.46
 C      -0.263726     0.748264    -0.240903      44.76
 H       0.828408     0.588286    -0.288358      17.80
 C      -2.515180    -0.044277    -0.647702      10.43
 C      -3.646215    -1.235929    -0.946746      80.90
 H      -4.572270    -0.767365    -1.092325      24.83
 O      -3.011618    -1.920654    -2.084118     283.44
 H      -3.335114    -2.925052    -2.043588      18.75
 C      -4.007649    -2.077112     0.292308      84.79
 H      -3.041366    -2.466585     0.814215      20.07
 O      -4.795811    -1.440403     1.297113     344.02
 H      -4.748756    -1.731638     2.160467      30.54
 C      -4.919523    -3.342015    -0.003649      75.15
 O      -4.164411    -4.373352    -0.870695     277.34
 H      -3.699838    -4.934185    -0.163193      26.31
 H      -5.892853    -3.120847    -0.703322      26.06
 H      -4.986463    -3.600105     1.025985      28.75
55
name = lig-etoh-frame_333
 C       2.764011     1.907807    -1.984366      73.16
 H       2.185000     2.655143    -2.561141      22.42
 C       3.999677     1.468457     0.097137      64.38
 H       4.138536     1.553627     1.078873      24.05
 C       4.605148     0.342324    -0.581724      19.20
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 O       5.332828    -0.667210     0.085373     269.57
 C       5.471707    -0.473249     1.532353     118.04
 H       4.559566    -0.334990     2.019004      29.09
 H       6.212538     0.240691     1.843129      28.69
 H       5.721286    -1.481414     1.678896      26.12
 C       4.142961    -0.103010    -1.855090      42.98
 O       4.363079    -1.274913    -2.376987     239.90
 H       5.149948    -1.569313    -2.040120      27.98
 C       3.294882     0.784600    -2.600598      46.82
 H       3.020404     0.342687    -3.690687      20.35
 C       3.115718     2.264752    -0.611666      28.28
 C       2.548116     3.660613    -0.133110      90.52
 H       2.877233     4.493172    -0.860026      21.44
 O       2.744244     4.079049     1.249420     252.86
 H       3.776618     4.308210     1.368160      26.71
 C       0.874028     3.773430    -0.311647      50.04
 H       0.812620     3.385303    -1.426947      17.67
 C       0.126764     5.193433    -0.219652     101.25
 O       0.813977     6.263360    -1.132500     234.35
 H       0.340414     5.970731    -1.905907      29.02
 H       0.256443     5.459343     0.890423      24.45
 H      -0.967320     5.036023    -0.081644      23.50
 C      -1.112844    -0.225824    -0.699639      44.55
 H      -0.572417    -1.004201    -1.361302      18.83
 C      -2.983587     1.160416     0.037889      60.70
 H      -4.022394     1.295286    -0.341492      21.47
 C      -2.125057     2.189021     0.384321       6.72
 O      -2.533605     3.503242     0.604278     181.21
 C      -3.919026     3.677834     1.211238     116.55
 H      -4.611460     4.198026     0.551519      27.01
 H      -4.526606     2.698948     1.102144      23.47
 H      -3.782447     4.359966     2.139045      25.13
 C      -0.611479     1.978058     0.313760       9.31
 O       0.403119     2.824129     0.759706     162.45
 C      -0.292701     0.754788    -0.216873      36.71
 H       0.869233     0.742963    -0.098076      15.69
 C      -2.604178    -0.047912    -0.612078      13.87
 C      -3.558693    -1.216406    -0.913669      80.20
 H      -4.682172    -0.839918    -1.167486      22.24
 O      -3.041025    -1.933167    -2.077303     282.75
 H      -3.423907    -2.857262    -2.284254      22.73
 C      -4.013579    -2.112177     0.247628      90.35
 H      -3.122146    -2.526503     0.615140      23.40
 O      -4.817837    -1.458884     1.322838     299.74
 H      -4.749643    -1.730943     2.292716      26.15
 C      -4.933695    -3.469641    -0.035205      80.19
 O      -4.185926    -4.361271    -0.806664     333.41
 H      -3.703346    -4.841087    -0.151906      29.77
 H      -5.694138    -2.964752    -0.516195      30.47
 H      -5.387585    -3.578242     1.044284      28.08
55
name = lig-etoh-frame_334
 C       2.810047     1.947661    -2.040126      32.90
 H       2.114069     2.520739    -2.658824      19.93
 C       4.028325     1.516200     0.000703      32.11
 H       4.118495     1.667565     1.188382      16.84
 C       4.552276     0.350355    -0.562084      22.20
 O       5.344648    -0.674758     0.070975     255.11
 C       5.519436    -0.438579     1.543734      98.84
 H       4.505948    -0.341735     2.143777      25.32
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 H       6.329886     0.333567     1.764985      26.45
 H       5.771256    -1.544816     1.888918      24.57
 C       4.158435    -0.055401    -1.790174      24.16
 O       4.318537    -1.282212    -2.386042     192.32
 H       5.203353    -1.761056    -2.082050      23.50
 C       3.168228     0.786405    -2.666011      71.29
 H       3.071113     0.890343    -3.724873      29.30
 C       3.081716     2.279217    -0.620396      77.52
 C       2.547281     3.702306    -0.056307      86.47
 H       3.148013     4.728861    -0.572238      22.82
 O       2.784589     4.083426     1.329877     236.70
 H       3.727653     4.386790     1.133048      26.60
 C       0.885094     3.773357    -0.398290      46.97
 H       0.572149     3.321925    -1.297150      22.11
 C       0.143406     5.233252    -0.245389     101.56
 O       0.833317     6.272406    -1.079277     186.54
 H       0.347542     6.127342    -2.000270      26.61
 H       0.546899     5.525792     0.742149      24.49
 H      -0.947661     5.119810    -0.492878      23.47
 C      -1.163798    -0.282784    -0.670804      34.64
 H      -0.567035    -0.779830    -1.467374      18.61
 C      -3.046929     1.189717     0.004667      47.88
 H      -3.985097     1.613168    -0.343460      20.47
 C      -2.113167     2.155931     0.394582      -7.65
 O      -2.520469     3.574188     0.614078     174.41
 C      -3.910238     3.599938     1.157282     108.75
 H      -4.539861     4.222765     0.405472      25.09
 H      -4.307541     2.618567     1.351543      25.04
 H      -3.946444     4.121716     2.188775      25.81
 C      -0.641665     1.982919     0.403747       5.03
 O       0.420705     2.796003     0.756020     154.08
 C      -0.246817     0.774188    -0.173401      19.82
 H       0.780404     0.576542    -0.181320      16.35
 C      -2.598500    -0.082293    -0.546502      15.71
 C      -3.554914    -1.171040    -0.911561      88.85
 H      -4.387684    -0.739414    -1.365786      23.44
 O      -3.062210    -1.944761    -2.074143     298.16
 H      -3.570606    -2.681706    -2.247153      25.84
 C      -4.015587    -2.214879     0.284013      68.85
 H      -2.982951    -2.650286     0.672036      19.06
 O      -4.844506    -1.447672     1.322418     265.62
 H      -4.329168    -1.825870     2.213364      21.78
 C      -4.933125    -3.475070    -0.039786      91.96
 O      -4.212992    -4.384850    -0.744683     315.43
 H      -3.555084    -4.851495    -0.107699      26.85
 H      -5.820086    -2.978880    -0.679328      26.13
 H      -5.550194    -3.973980     0.721459      26.26
55
name = lig-etoh-frame_335
 C       2.814208     2.024220    -2.059211      42.94
 H       2.100575     2.598287    -2.656671      20.72
 C       4.051500     1.561090    -0.016553      25.72
 H       4.255646     1.853443     0.960200      19.09
 C       4.513335     0.318237    -0.521417      13.99
 O       5.348268    -0.649146     0.086996     263.99
 C       5.559052    -0.465120     1.557547     119.33
 H       4.672869    -0.127078     2.013492      29.03
 H       6.268304     0.319166     1.692354      28.65
 H       5.999140    -1.272570     2.055826      27.58
 C       4.075832     0.015653    -1.850890      10.74
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 O       4.305784    -1.312662    -2.398475     196.91
 H       5.020120    -1.969147    -2.048931      22.40
 C       3.130245     0.781938    -2.661385      81.44
 H       3.125122     0.997638    -3.784032      27.57
 C       3.033269     2.353388    -0.683094      54.01
 C       2.498912     3.762899    -0.034788     104.84
 H       3.188873     4.459318    -0.500230      25.14
 O       2.831885     4.069840     1.393458     270.01
 H       3.719486     4.387156     1.333258      30.35
 C       0.924450     3.788576    -0.430170      34.23
 H       0.398771     3.168200    -1.302495      18.00
 C       0.226846     5.242441    -0.273389     100.26
 O       0.819472     6.256828    -1.030623     194.11
 H       0.730779     6.334713    -2.115878      26.80
 H       0.498783     5.657296     0.802081      23.20
 H      -0.756905     5.276724    -0.707602      23.58
 C      -1.196657    -0.270560    -0.632931      38.43
 H      -0.820620    -0.962141    -1.390213      19.27
 C      -3.083113     1.200190    -0.065032      47.93
 H      -4.076510     1.750228    -0.147491      17.48
 C      -2.059814     2.202651     0.412148     -13.96
 O      -2.524843     3.598837     0.638310     191.99
 C      -3.899033     3.552652     1.094011     109.31
 H      -4.443648     4.092866     0.395698      25.89
 H      -4.096509     2.499250     1.604363      22.92
 H      -3.990530     3.997762     2.155402      25.17
 C      -0.706784     1.949035     0.474738       6.61
 O       0.421403     2.807789     0.744516     128.28
 C      -0.239545     0.747523    -0.130881      19.74
 H       0.857973     0.355625    -0.406436      14.07
 C      -2.545729    -0.116558    -0.462724      22.24
 C      -3.595269    -1.168163    -0.932155      53.37
 H      -4.430512    -0.458454    -1.415211      20.72
 O      -3.056114    -1.944864    -2.068665     222.39
 H      -3.838443    -2.650748    -2.126675      20.62
 C      -4.024787    -2.302124     0.362557      71.09
 H      -3.125874    -2.608127     0.789670      20.77
 O      -4.817250    -1.459552     1.323688     338.33
 H      -4.234231    -1.612392     1.988563      26.65
 C      -4.983187    -3.398143    -0.058430     104.59
 O      -4.209239    -4.464468    -0.718206     312.61
 H      -3.508558    -4.775300    -0.077814      26.65
 H      -5.671959    -3.257070    -0.847595      27.25
 H      -5.483167    -4.137940     0.658760      23.79
55
name = lig-etoh-frame_336
 C       2.763970     2.111340    -2.056486      59.59
 H       2.163604     2.841344    -2.637070      19.61
 C       4.041648     1.610375    -0.024861      34.57
 H       4.489128     2.061553     0.953704      15.12
 C       4.459901     0.297488    -0.503481      11.69
 O       5.345897    -0.619096     0.120268     236.62
 C       5.603696    -0.459359     1.544370      99.82
 H       4.652566     0.022977     1.988232      24.54
 H       6.301119     0.465839     1.615138      26.60
 H       6.199953    -1.299821     2.108075      24.39
 C       3.979445    -0.002167    -1.949922      15.30
 O       4.288679    -1.332443    -2.419250     218.98
 H       4.806339    -1.867324    -1.866850      23.06
 C       3.161041     0.828251    -2.623417      80.06
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 H       3.142870     0.563392    -3.729958      27.81
 C       3.029527     2.434442    -0.736601      55.57
 C       2.453701     3.763980    -0.054296      80.95
 H       3.133964     4.561413    -0.830430      21.48
 O       2.848057     4.034631     1.434487     240.06
 H       3.860599     4.329951     1.603930      26.57
 C       0.934595     3.801673    -0.394167      59.89
 H       0.740225     3.329513    -1.291197      20.21
 C       0.322056     5.223911    -0.301739     119.84
 O       0.856974     6.290984    -1.011699     293.70
 H       0.892744     6.095729    -1.883774      35.76
 H       0.168223     5.542509     0.755063      24.64
 H      -0.800277     5.167929    -0.518313      23.60
 C      -1.166811    -0.222884    -0.584924      46.36
 H      -1.080605    -1.315381    -1.029663      17.44
 C      -3.032911     1.232360    -0.111080      42.38
 H      -4.091492     1.374799    -0.037711      20.80
 C      -2.077816     2.275200     0.409970      -7.00
 O      -2.515927     3.574123     0.667937     210.23
 C      -3.866246     3.501438     1.107518     106.56
 H      -4.694056     3.837821     0.292678      24.50
 H      -4.137038     2.547851     1.357383      26.54
 H      -3.949096     4.277925     1.982166      24.20
 C      -0.682418     1.897187     0.502422       1.16
 O       0.397528     2.846837     0.739717     145.15
 C      -0.265070     0.644182    -0.122611      44.75
 H       0.710243     0.567860    -0.389144      16.69
 C      -2.577902    -0.111215    -0.382720       6.09
 C      -3.629418    -1.167151    -0.948979      57.32
 H      -4.491438    -0.590183    -1.109930      22.89
 O      -3.068459    -1.947561    -2.051063     249.66
 H      -3.786072    -2.656883    -2.181277      20.25
 C      -4.093979    -2.289342     0.406732      63.06
 H      -3.127581    -2.697775     0.946820      16.80
 O      -4.766436    -1.484738     1.314437     311.53
 H      -4.201285    -1.247186     2.241345      21.98
 C      -5.017306    -3.396268    -0.094682      79.74
 O      -4.177782    -4.560623    -0.715511     294.70
 H      -3.551620    -4.733385    -0.015127      27.91
 H      -5.703888    -3.201570    -0.987681      26.10
 H      -5.473079    -3.738779     0.893228      25.09
55
name = lig-etoh-frame_337
 C       2.697077     2.181342    -2.070217      55.54
 H       2.266494     2.943831    -2.702735      20.97
 C       4.018197     1.637096    -0.030206      33.41
 H       4.611171     2.101082     0.783387      19.77
 C       4.376936     0.326653    -0.529589      18.80
 O       5.329508    -0.597294     0.136882     243.67
 C       5.659745    -0.375486     1.536096     121.36
 H       4.743855    -0.203767     2.096402      26.91
 H       6.325589     0.441026     1.582876      27.59
 H       6.044699    -1.299243     1.853224      26.50
 C       3.937901    -0.105928    -1.929572      18.44
 O       4.256077    -1.324101    -2.458871     187.93
 H       4.684491    -1.694146    -1.531680      19.01
 C       3.196866     0.912011    -2.619160      57.06
 H       2.948025     0.323287    -3.548122      20.16
 C       3.081929     2.495255    -0.735723      44.99
 C       2.496215     3.765521    -0.107453      91.54
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 H       2.607692     4.623120    -0.758491      23.60
 O       2.838725     3.990668     1.437817     255.09
 H       3.813516     4.117175     1.435377      28.54
 C       0.959104     3.813698    -0.286885      42.52
 H       1.064985     3.476691    -1.443614      15.24
 C       0.331299     5.182530    -0.289960     104.83
 O       0.923191     6.340434    -0.992493     234.46
 H       0.939843     5.768743    -1.954640      26.86
 H       0.061211     5.402250     0.833834      22.54
 H      -0.716276     4.897386    -0.486775      22.64
 C      -1.211409    -0.300190    -0.541448      52.22
 H      -0.911395    -1.291408    -0.607284      19.87
 C      -2.949593     1.257805    -0.112515      61.24
 H      -4.079717     1.061101    -0.027621      18.21
 C      -2.093604     2.291640     0.376483       1.93
 O      -2.497811     3.528443     0.697663     212.74
 C      -3.882893     3.520556     1.120596     115.90
 H      -4.570644     3.574248     0.340756      27.30
 H      -4.270201     2.405560     1.363689      22.95
 H      -3.967677     4.371675     1.780545      25.70
 C      -0.638574     1.875131     0.471167      -2.36
 O       0.349058     2.891987     0.734537     152.92
 C      -0.275982     0.608274    -0.090838      30.95
 H       0.878442     0.731479    -0.308050      13.09
 C      -2.633442    -0.062876    -0.349011      18.04
 C      -3.617534    -1.190087    -0.882948      49.15
 H      -4.743611    -0.797167    -0.992718      21.47
 O      -3.097676    -1.938638    -2.029453     281.50
 H      -3.558321    -2.692455    -2.282291      23.20
 C      -4.108820    -2.226089     0.406496      77.70
 H      -3.309569    -2.791143     0.794080      19.66
 O      -4.728799    -1.489353     1.343968     367.34
 H      -4.342084    -1.057398     2.162906      27.01
 C      -5.021859    -3.443223    -0.137663      69.51
 O      -4.162777    -4.631385    -0.701701     273.01
 H      -3.548032    -4.815595     0.131206      25.55
 H      -5.755154    -3.016156    -0.834375      28.17
 H      -5.610374    -3.448472     0.842369      25.77
55
name = lig-etoh-frame_338
 C       2.681090     2.198526    -2.085977      90.74
 H       2.271939     2.924706    -2.833332      24.49
 C       3.992356     1.635790    -0.064565      47.41
 H       4.581053     1.991649     0.758762      23.34
 C       4.310133     0.356534    -0.576679       7.08
 O       5.280818    -0.558530     0.120742     213.43
 C       5.687729    -0.293308     1.512929     103.12
 H       4.825128    -0.330672     2.261568      25.22
 H       6.497432     0.520161     1.688030      24.69
 H       6.069297    -1.379860     1.676892      24.01
 C       3.891760    -0.122157    -1.821947      27.40
 O       4.230446    -1.314153    -2.462090     234.17
 H       4.606501    -1.797346    -1.688959      24.44
 C       3.224380     0.961667    -2.623258      36.88
 H       2.533009     0.538466    -3.464363      19.12
 C       3.154077     2.543018    -0.731147      18.33
 C       2.526920     3.766820    -0.090891      90.69
 H       2.633668     4.960562    -0.696344      17.64
 O       2.819789     3.938975     1.377674     275.86
 H       3.815926     3.992518     1.252058      26.17
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 C       1.032476     3.783651    -0.209461      69.76
 H       0.884614     3.524984    -1.202471      20.22
 C       0.271920     5.147040    -0.196273      94.60
 O       0.973394     6.319122    -0.995639     145.85
 H       0.957932     5.988474    -1.962948      29.46
 H       0.281752     5.470000     0.817511      24.75
 H      -0.639890     4.880600    -0.819688      22.76
 C      -1.285655    -0.428186    -0.461868      31.96
 H      -0.642228    -1.417476    -0.442657      17.16
 C      -2.940098     1.264374    -0.078853      57.99
 H      -4.003763     1.413336    -0.042723      22.09
 C      -2.038528     2.231066     0.328338      10.46
 O      -2.488002     3.488938     0.737748     196.25
 C      -3.924759     3.504189     1.123351      96.74
 H      -4.465933     3.614379     0.068362      23.81
 H      -4.133123     2.701599     1.773457      26.56
 H      -4.148629     4.500948     1.806548      23.95
 C      -0.645571     1.909626     0.384041      11.42
 O       0.287803     2.931803     0.725285     211.24
 C      -0.240484     0.659851    -0.047508      25.12
 H       0.808787     0.460471    -0.152883      16.18
 C      -2.616639    -0.065399    -0.393201      38.61
 C      -3.648168    -1.235819    -0.755153      82.68
 H      -4.580888    -0.909052    -1.119182      22.37
 O      -3.111495    -1.894821    -2.002038     244.92
 H      -3.484802    -2.867892    -2.236606      19.22
 C      -4.050864    -2.190042     0.338817      86.64
 H      -3.161066    -2.839637     0.708512      18.14
 O      -4.753352    -1.461994     1.387746     374.93
 H      -4.175044    -1.186985     2.059318      30.29
 C      -4.999614    -3.457492    -0.161700      78.85
 O      -4.178516    -4.658537    -0.651273     284.30
 H      -3.668065    -4.971149     0.118867      28.26
 H      -5.726048    -3.058632    -0.914707      27.63
 H      -5.769647    -3.706190     0.671533      25.80
55
name = lig-etoh-frame_339
 C       2.744818     2.181047    -2.084419     116.22
 H       2.183498     2.799981    -2.768087      25.64
 C       3.971392     1.634072    -0.106873      45.63
 H       4.463021     1.818686     0.963793      20.61
 C       4.301344     0.358013    -0.582426      19.45
 O       5.203670    -0.487124     0.090721     231.79
 C       5.710530    -0.270520     1.490175     120.36
 H       4.949784    -0.182497     2.280604      27.02
 H       6.425411     0.483367     1.708865      28.04
 H       6.304327    -1.155787     1.622405      26.64
 C       3.812185    -0.051703    -1.772869      44.51
 O       4.199807    -1.299381    -2.438084     237.46
 H       4.659325    -2.063415    -1.996860      25.78
 C       3.184633     0.966936    -2.610602      44.45
 H       2.533761     0.843903    -3.449198      20.13
 C       3.197546     2.593333    -0.773507       1.69
 C       2.548342     3.828518    -0.045017     114.78
 H       2.987085     4.670710    -0.394440      19.88
 O       2.818946     3.882476     1.282186     290.94
 H       3.878907     4.021801     1.393876      25.23
 C       1.060942     3.749773    -0.174026      63.18
 H       0.612371     3.299811    -1.175496      17.52
 C       0.238328     5.127599    -0.135665      90.49
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 O       1.003464     6.256251    -0.988673     154.35
 H       0.912120     6.196224    -1.935071      30.36
 H       0.289755     5.743285     0.894136      22.58
 H      -0.599637     5.126195    -0.791111      23.44
 C      -1.239777    -0.498399    -0.325685      28.23
 H      -0.882956    -1.473262    -0.520332      15.77
 C      -2.980360     1.247801    -0.045249      59.76
 H      -3.932863     1.854992    -0.080710      11.91
 C      -1.993448     2.178610     0.294695      14.57
 O      -2.480147     3.453306     0.792345     177.05
 C      -3.954747     3.530696     1.109145     116.57
 H      -4.455964     3.557660     0.201132      26.90
 H      -4.124133     2.867467     2.073388      23.62
 H      -4.167069     4.427539     1.593641      27.28
 C      -0.635862     1.980920     0.263799      21.37
 O       0.228340     2.961172     0.736983     234.10
 C      -0.255387     0.655259    -0.027324      33.63
 H       0.765206     0.221217     0.011139      15.52
 C      -2.596064    -0.136358    -0.460334      19.42
 C      -3.678104    -1.258803    -0.682328      86.42
 H      -4.556361    -0.686106    -1.192525      22.93
 O      -3.111754    -1.858538    -1.977184     274.32
 H      -3.425379    -2.796903    -1.895929      22.49
 C      -3.986843    -2.236770     0.303410      79.21
 H      -3.050655    -2.595793     0.711565      22.76
 O      -4.787152    -1.434475     1.417506     298.63
 H      -3.869431    -1.500804     2.061977      19.93
 C      -4.972295    -3.457111    -0.178474      86.57
 O      -4.223424    -4.651286    -0.597411     286.13
 H      -3.766319    -5.064387     0.188889      26.98
 H      -5.483147    -3.296721    -1.177116      27.76
 H      -5.634641    -3.983626     0.547308      25.42
55
name = lig-etoh-frame_340
 C       2.843809     2.185277    -2.059475      44.23
 H       2.066553     2.756522    -2.613591      21.55
 C       3.967032     1.650860    -0.091456      80.80
 H       4.159823     1.782690     0.898731      22.21
 C       4.320212     0.378857    -0.535758      20.80
 O       5.136648    -0.422501     0.079443     234.76
 C       5.726718    -0.263027     1.452182     109.23
 H       4.934601    -0.093900     2.213209      27.37
 H       6.358217     0.729747     1.493463      27.50
 H       6.462891    -1.094383     1.640440      25.01
 C       3.745974    -0.021243    -1.824845      40.31
 O       4.144138    -1.260074    -2.414802     211.18
 H       4.762500    -2.100337    -2.177739      24.36
 C       3.103617     0.939910    -2.577615      69.44
 H       2.799901     0.788119    -3.738711      22.43
 C       3.213438     2.624754    -0.824387      31.43
 C       2.587249     3.832688    -0.041962      98.40
 H       3.260783     4.833462    -0.583715      15.01
 O       2.855355     3.824999     1.267053     335.19
 H       3.698102     4.076180     1.489808      32.50
 C       0.967850     3.752102    -0.208909      59.88
 H       0.789562     3.231216    -1.136401      19.37
 C       0.281375     5.175574    -0.121529     110.46
 O       1.038108     6.178226    -0.947882     162.72
 H       0.633613     6.211337    -2.018193      23.69
 H       0.092462     5.644385     0.772216      26.62
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 H      -0.833932     5.186332    -0.448484      23.64
 C      -1.171028    -0.469734    -0.188129      42.42
 H      -1.042231    -1.571019    -0.564765      15.18
 C      -3.000934     1.192387    -0.041979      55.66
 H      -3.948304     1.731642    -0.225814      18.06
 C      -2.024335     2.176821     0.284885      -1.22
 O      -2.475084     3.416443     0.847566     160.74
 C      -3.928896     3.549544     1.135145     104.02
 H      -4.732141     3.298824     0.277515      23.94
 H      -4.306002     2.879514     1.904401      26.11
 H      -4.044568     4.775622     1.337748      23.80
 C      -0.587425     2.014058     0.145358      15.15
 O       0.189531     2.978190     0.783984     217.09
 C      -0.295488     0.570134    -0.025763      34.38
 H       0.807834     0.309917     0.233134      15.53
 C      -2.605236    -0.182655    -0.462389       8.11
 C      -3.682839    -1.184265    -0.748336      87.68
 H      -4.582915    -0.575515    -0.892740      24.11
 O      -3.114854    -1.846811    -1.937533     290.11
 H      -3.300331    -2.744727    -1.770440      23.14
 C      -4.003454    -2.312903     0.335574      62.27
 H      -3.000125    -2.549402     0.807595      19.35
 O      -4.752656    -1.437181     1.435305     299.89
 H      -4.227924    -1.680889     2.213450      25.27
 C      -4.913210    -3.475291    -0.215378      88.03
 O      -4.249849    -4.652027    -0.558812     284.27
 H      -3.788469    -5.044820     0.290700      25.35
 H      -5.342908    -3.277451    -1.174535      28.45
 H      -5.670898    -3.822787     0.642393      25.17
55
name = lig-etoh-frame_341
 C       2.887597     2.234042    -2.074466      84.14
 H       2.116320     2.824859    -2.552686      22.63
 C       3.957844     1.688214    -0.056011      25.61
 H       3.966163     1.962136     1.121151      14.77
 C       4.281617     0.448337    -0.540515      16.93
 O       5.119687    -0.427844     0.107317     255.20
 C       5.744401    -0.199112     1.390290     111.00
 H       4.912704    -0.184811     2.151615      27.34
 H       6.140309     0.765362     1.213415      27.48
 H       6.397903    -1.065400     1.613347      25.32
 C       3.759656    -0.041380    -1.855246      15.84
 O       4.067901    -1.225515    -2.424333     227.74
 H       4.772136    -1.644778    -1.949207      24.93
 C       3.020350     0.883792    -2.606885      99.52
 H       3.093155     0.611143    -3.588937      32.35
 C       3.234149     2.620362    -0.812685      59.25
 C       2.644287     3.837872    -0.134224      96.08
 H       2.864413     4.679498    -0.646705      23.92
 O       2.883237     3.765851     1.325947     299.77
 H       3.856964     4.212356     1.488835      27.13
 C       0.875947     3.810765    -0.246107      38.63
 H       0.879503     3.337732    -1.288728      17.54
 C       0.306540     5.236639    -0.168673     113.50
 O       1.048685     6.102612    -0.924658     279.67
 H       0.530434     6.003414    -1.663548      31.70
 H       0.196349     5.484871     1.052450      24.18
 H      -0.769253     5.052153    -0.214642      24.75
 C      -1.199675    -0.460623    -0.116706      57.73
 H      -0.839936    -1.483665    -0.354477      17.32
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 C      -2.988900     1.113474    -0.080946      53.44
 H      -4.075090     1.248148    -0.315919      19.55
 C      -2.059604     2.195412     0.281962      -2.92
 O      -2.486747     3.370674     0.892740     189.98
 C      -3.913047     3.594179     1.128874     136.20
 H      -4.557616     3.161610     0.432969      27.69
 H      -4.349399     2.908008     1.969617      25.79
 H      -4.100102     4.531208     1.205736      29.83
 C      -0.614896     1.974971     0.073594      14.51
 O       0.179847     2.978743     0.823877     183.91
 C      -0.262463     0.535440     0.006628      37.17
 H       0.730416     0.467947     0.274091      16.93
 C      -2.594893    -0.142277    -0.372300      21.13
 C      -3.661620    -1.117408    -0.819119      65.42
 H      -4.713915    -0.620141    -0.800395      23.07
 O      -3.131572    -1.842627    -1.909594     252.79
 H      -3.157806    -2.907972    -1.801667      18.76
 C      -4.040266    -2.313893     0.401050      58.03
 H      -3.110518    -2.747896     0.844230      20.09
 O      -4.701559    -1.477878     1.430479     271.81
 H      -4.543896    -1.754349     2.427524      24.73
 C      -4.870828    -3.478366    -0.214972      82.28
 O      -4.244663    -4.688838    -0.530301     318.31
 H      -3.695813    -4.938480     0.230831      30.16
 H      -5.467003    -2.980400    -1.089983      27.54
 H      -5.724103    -3.397654     0.571064      25.84
55
name = lig-etoh-frame_342
 C       2.875022     2.260958    -2.149173      62.44
 H       2.304639     3.018344    -2.727378      19.89
 C       3.939595     1.742109     0.037299      19.54
 H       4.015794     1.999810     0.998665      17.39
 C       4.233359     0.486826    -0.574256       3.35
 O       5.108844    -0.488314     0.120013     245.46
 C       5.716793    -0.121008     1.318856     110.19
 H       5.000370    -0.196597     2.152699      27.24
 H       6.216918     0.924844     1.245127      26.08
 H       6.407617    -0.946340     1.516385      25.71
 C       3.788464    -0.003580    -1.833590      16.35
 O       4.004807    -1.214261    -2.433313     202.44
 H       4.770263    -1.326607    -1.722678      20.31
 C       2.979517     0.857349    -2.607064      62.09
 H       3.074218     0.487779    -3.768822      27.32
 C       3.249080     2.602716    -0.779897      47.46
 C       2.616412     3.794891    -0.181683      79.68
 H       2.694858     4.942095    -0.757079      18.21
 O       2.932665     3.740457     1.374568     294.40
 H       3.827509     4.187214     1.360375      28.40
 C       0.856157     3.857923    -0.266710      41.07
 H       0.625052     3.518681    -1.342330      16.44
 C       0.304749     5.224106    -0.087141     116.04
 O       1.047328     6.059010    -0.917542     185.97
 H       0.546124     5.946695    -1.867977      26.74
 H       0.630041     5.388475     0.864689      26.43
 H      -0.784278     5.153232    -0.418095      23.77
 C      -1.237853    -0.478813    -0.090351      49.90
 H      -0.702179    -1.465452    -0.069772      17.37
 C      -2.994616     1.120667    -0.126841      62.53
 H      -4.105238     0.941260    -0.198790      19.58
 C      -2.093372     2.184844     0.263810       8.97
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 O      -2.501689     3.332330     0.929864     191.83
 C      -3.901072     3.548814     1.128889     100.68
 H      -4.395030     3.090550     0.165017      23.76
 H      -4.119219     3.214701     2.189045      24.79
 H      -4.264285     4.785372     1.237544      23.57
 C      -0.717406     1.918232     0.091361      15.70
 O       0.186685     2.961841     0.799576     135.38
 C      -0.229784     0.588758     0.055814      23.36
 H       0.959449     0.431821     0.254446      14.28
 C      -2.552782    -0.134869    -0.265977      32.27
 C      -3.632143    -1.120899    -0.798681      62.67
 H      -4.650557    -0.750242    -1.077976      22.94
 O      -3.146652    -1.854657    -1.918674     281.52
 H      -3.167358    -2.811886    -1.759536      20.89
 C      -4.035436    -2.262448     0.464574      71.43
 H      -3.162628    -2.854265     0.830152      19.57
 O      -4.652419    -1.527684     1.413837     235.58
 H      -4.797016    -1.923656     2.424501      23.52
 C      -4.890131    -3.405399    -0.194012      74.05
 O      -4.250457    -4.723095    -0.520786     282.61
 H      -3.467306    -4.896433     0.205411      24.35
 H      -5.375351    -2.987736    -1.039913      28.19
 H      -5.810282    -3.354844     0.508195      26.15
55
name = lig-etoh-frame_343
 C       2.844976     2.246356    -2.223740      97.80
 H       2.626874     3.084319    -2.914539      17.69
 C       3.922859     1.740500     0.077438      36.49
 H       4.237764     1.993756     1.195441      14.56
 C       4.227753     0.475328    -0.558133      23.93
 O       5.067672    -0.547060     0.086318     236.31
 C       5.695891    -0.035217     1.272614     116.02
 H       5.059777    -0.053582     2.217332      26.59
 H       6.250078     0.883723     1.384626      30.30
 H       6.563002    -0.755275     1.437207      27.05
 C       3.757441     0.098097    -1.818561      29.64
 O       3.988125    -1.212133    -2.395428     183.39
 H       4.779626    -1.684246    -1.851080      21.57
 C       2.983680     0.905065    -2.630041      19.97
 H       2.698389     0.639817    -3.566361      28.59
 C       3.216980     2.599904    -0.809774     100.76
 C       2.508024     3.790852    -0.173552      99.72
 H       2.829903     4.743194    -0.519497      14.77
 O       2.969850     3.748270     1.365185     271.53
 H       3.907115     4.130588     1.352235      29.88
 C       0.874461     3.822778    -0.279959      59.64
 H       0.424871     3.559601    -1.258996      16.21
 C       0.295303     5.171916     0.010118      98.01
 O       1.029999     6.061321    -0.960980     164.47
 H       0.947284     5.953591    -2.024253      26.15
 H       0.824081     5.606623     1.023945      21.95
 H      -0.705796     5.414048    -0.321465      23.40
 C      -1.162161    -0.475361    -0.069227      40.45
 H      -0.843392    -1.586907     0.215803      18.38
 C      -3.032218     1.187201    -0.152658      71.48
 H      -4.089291     1.273655     0.015163      23.66
 C      -2.165730     2.157672     0.244403      11.22
 O      -2.495842     3.315223     0.958044     211.88
 C      -3.911097     3.535861     1.126874     134.06
 H      -4.400306     3.104455     0.278310      27.17
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 H      -4.099437     3.277559     2.184263      26.42
 H      -4.073441     4.515668     1.073368      29.08
 C      -0.779508     1.900025     0.196316       9.23
 O       0.189786     2.927461     0.712552     172.37
 C      -0.225288     0.631357     0.102642      35.06
 H       0.742775     0.448518     0.134770      18.07
 C      -2.529661    -0.202127    -0.209130      39.42
 C      -3.588394    -1.200645    -0.706499      73.15
 H      -4.471585    -0.672525    -1.223153      21.80
 O      -3.148032    -1.869571    -1.948363     285.26
 H      -3.240756    -2.784012    -1.695198      22.78
 C      -3.979840    -2.234537     0.457462      82.31
 H      -3.020556    -2.748985     0.816467      18.73
 O      -4.645316    -1.547443     1.430981     295.56
 H      -4.716787    -2.091455     2.116494      28.93
 C      -4.938661    -3.326301    -0.160552      66.12
 O      -4.265071    -4.719119    -0.508446     255.80
 H      -3.519842    -4.884638     0.080187      27.38
 H      -5.235697    -3.124895    -1.279220      25.12
 H      -5.825482    -3.676496     0.541814      25.45
55
name = lig-etoh-frame_344
 C       2.835905     2.254269    -2.235228     124.83
 H       2.744651     3.004412    -2.990737      32.36
 C       3.902961     1.696206     0.062950      79.19
 H       4.330624     1.928848     1.012866      19.05
 C       4.249293     0.449753    -0.501486       4.01
 O       5.011915    -0.564881     0.043901     215.91
 C       5.709955     0.007937     1.275245     111.36
 H       5.050265     0.029037     2.123342      27.02
 H       6.163058     1.067637     1.158399      30.01
 H       6.513770    -0.641507     1.451318      27.36
 C       3.724082     0.133188    -1.816833      43.55
 O       3.993255    -1.209198    -2.334243     250.90
 H       4.558207    -1.884157    -2.108109      27.13
 C       2.998927     1.007346    -2.657521      40.99
 H       2.285026     0.668461    -3.571756      16.91
 C       3.147376     2.599725    -0.862851      99.19
 C       2.408947     3.760731    -0.100326     123.55
 H       2.985437     4.820643    -0.474256      12.98
 O       2.966158     3.777155     1.314003     299.63
 H       4.012411     4.050710     1.296819      28.29
 C       0.877143     3.746487    -0.264446      58.02
 H       0.463114     3.503979    -1.351604      17.01
 C       0.355148     5.184936     0.078404      98.91
 O       1.032773     6.098059    -1.016929     208.64
 H       0.999303     5.750705    -1.851252      32.27
 H       0.525677     5.675166     0.958498      25.56
 H      -0.749991     5.399665     0.107499      24.34
 C      -1.080151    -0.475442    -0.024069      42.34
 H      -0.932929    -1.485788     0.207247      17.89
 C      -3.079657     1.184737    -0.164682      57.64
 H      -4.090972     1.639706     0.124401      19.79
 C      -2.207673     2.165076     0.260012      11.93
 O      -2.483844     3.306370     0.967947     198.57
 C      -3.899037     3.519904     1.131494     113.01
 H      -4.675272     3.003998     0.457923      23.82
 H      -4.376228     3.094041     2.144776      24.62
 H      -3.964149     4.741000     0.896954      23.64
 C      -0.763958     1.923687     0.332704      16.46
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 O       0.180958     2.870148     0.616027     218.06
 C      -0.290223     0.638001     0.133812      34.46
 H       0.915647     0.518038     0.092364      13.82
 C      -2.530911    -0.234025    -0.193075      19.09
 C      -3.541488    -1.283791    -0.616491      80.48
 H      -4.303598    -0.503470    -0.913300      21.75
 O      -3.133729    -1.898884    -1.968397     216.95
 H      -3.268915    -2.963769    -1.789459      19.06
 C      -3.918430    -2.241660     0.378814      83.14
 H      -2.960073    -2.593178     0.780213      18.85
 O      -4.658061    -1.532114     1.458734     206.58
 H      -4.596399    -2.328669     2.184451      24.45
 C      -4.969104    -3.312130    -0.160792      84.37
 O      -4.293909    -4.678827    -0.510705     241.80
 H      -3.560058    -4.905975     0.179864      25.19
 H      -5.261745    -3.129235    -1.142565      28.25
 H      -5.735979    -3.828957     0.486470      26.09
55
name = lig-etoh-frame_345
 C       2.840529     2.346812    -2.182795      87.74
 H       2.490245     3.077056    -2.960014      26.13
 C       3.859042     1.651204    -0.033688      62.48
 H       4.237866     2.011283     0.941598      18.36
 C       4.241447     0.426063    -0.502776      11.89
 O       4.980102    -0.553111     0.041890     242.28
 C       5.731787     0.046288     1.263503      90.71
 H       4.925468     0.088730     2.079140      25.01
 H       5.927399     1.002267     0.788049      26.77
 H       6.548013    -0.722441     1.548703      24.28
 C       3.721583     0.080328    -1.812551      18.05
 O       3.958425    -1.173302    -2.301725     199.33
 H       4.594447    -2.000869    -1.992809      21.87
 C       3.010412     1.020098    -2.709497      79.95
 H       2.365646     0.673070    -3.439481      21.57
 C       3.079871     2.586700    -0.861471      46.66
 C       2.419421     3.736842    -0.036080     115.97
 H       2.658980     4.677334    -0.595633      22.07
 O       2.931269     3.808625     1.256339     330.31
 H       3.834173     4.003283     1.148528      31.35
 C       0.848807     3.716606    -0.243376      56.90
 H       0.763332     3.504031    -1.316308      19.24
 C       0.417440     5.241010     0.068198      89.00
 O       1.019991     6.142316    -1.028459     150.77
 H       0.801974     5.367300    -1.834612      23.98
 H       0.663600     5.695195     1.158846      22.79
 H      -0.676063     5.045290     0.193896      23.36
 C      -1.122394    -0.462068     0.017431      43.14
 H      -0.686867    -1.644162     0.044077      16.54
 C      -3.095702     1.140759    -0.138951      49.61
 H      -4.130568     1.379590    -0.094357      21.36
 C      -2.154030     2.166826     0.306406      13.91
 O      -2.509802     3.305241     0.967176     200.68
 C      -3.926055     3.541702     1.144238     135.60
 H      -4.676924     3.048425     0.515767      26.46
 H      -4.336012     3.199328     2.072587      27.33
 H      -4.102080     4.597660     0.980102      27.11
 C      -0.759446     1.928815     0.422423      27.44
 O       0.183708     2.816649     0.567961     227.63
 C      -0.287177     0.634953     0.163466      37.92
 H       0.745135     0.673666     0.160612      18.12
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 C      -2.510007    -0.210155    -0.190476      29.97
 C      -3.480426    -1.281738    -0.610186      79.12
 H      -4.438105    -0.679037    -0.640355      23.03
 O      -3.121143    -1.951712    -1.957908     266.14
 H      -3.231741    -2.873435    -2.020481      24.90
 C      -3.921027    -2.290156     0.345210      83.59
 H      -2.970052    -2.736406     0.839351      18.66
 O      -4.665078    -1.538087     1.483011     192.72
 H      -4.455032    -2.139081     2.350138      23.36
 C      -4.936204    -3.374559    -0.166576      76.44
 O      -4.309158    -4.623707    -0.522989     279.47
 H      -3.729837    -4.889524     0.277285      27.82
 H      -5.558597    -2.891854    -1.092772      26.35
 H      -5.789247    -3.538595     0.601374      26.78
55
name = lig-etoh-frame_346
 C       2.828792     2.420164    -2.173212      32.38
 H       2.141142     3.135877    -2.624062      17.37
 C       3.802365     1.646747    -0.132435      42.86
 H       3.978489     2.088387     0.923883      16.31
 C       4.193189     0.398716    -0.585309      18.63
 O       4.982704    -0.549993     0.085879     263.68
 C       5.710938     0.045402     1.223793     112.79
 H       5.014680     0.227878     2.005750      27.58
 H       6.048657     0.997608     0.768627      27.33
 H       6.480154    -0.582489     1.553752      26.96
 C       3.714759     0.035128    -1.833851      18.25
 O       3.913927    -1.180075    -2.308349     212.97
 H       4.560529    -1.546421    -1.623923      22.04
 C       3.060554     1.005506    -2.679899      99.32
 H       2.531517     0.591541    -3.655161      23.61
 C       3.039272     2.569710    -0.790094      65.80
 C       2.435742     3.685664    -0.046589      97.17
 H       2.499691     4.781905    -0.802094      19.75
 O       2.870516     3.844231     1.226196     274.83
 H       3.937783     4.080222     1.122581      25.33
 C       0.869590     3.754570    -0.208954      40.68
 H       0.925365     3.511498    -1.360463      14.99
 C       0.466869     5.286636     0.061938     115.22
 O       0.965387     6.131364    -1.024556     203.02
 H       0.646615     5.656278    -1.823423      29.66
 H       1.021236     5.500285     0.938861      25.55
 H      -0.602445     5.055912    -0.036257      23.62
 C      -1.179193    -0.485664     0.042997      52.17
 H      -0.704607    -1.321890    -0.173488      18.97
 C      -3.029933     1.089104    -0.077359      59.04
 H      -4.146368     0.961174    -0.396174      17.79
 C      -2.124680     2.135469     0.371095      23.58
 O      -2.565558     3.328473     0.959689     183.45
 C      -3.976361     3.558631     1.152832     104.94
 H      -4.503717     3.035230     0.320767      23.91
 H      -4.132489     3.360362     2.358541      23.05
 H      -4.286934     4.707710     1.112034      24.73
 C      -0.789376     1.869783     0.433572      30.24
 O       0.219989     2.804376     0.588509     201.78
 C      -0.280685     0.628413     0.204379      27.22
 H       0.882585     0.589535     0.242570      16.20
 C      -2.500356    -0.171605    -0.207051      41.03
 C      -3.455495    -1.257517    -0.661306      70.01
 H      -4.564959    -0.992045    -0.761324      22.28
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 O      -3.100963    -1.965652    -1.936237     274.37
 H      -3.323091    -2.928066    -1.999410      23.50
 C      -3.935162    -2.376429     0.411517      78.51
 H      -3.181973    -2.980983     0.851212      23.08
 O      -4.653016    -1.560325     1.492943     272.44
 H      -4.307195    -1.753875     2.339802      25.70
 C      -4.932545    -3.418293    -0.180415      95.00
 O      -4.328275    -4.570993    -0.543183     323.76
 H      -3.831121    -4.870092     0.214521      31.57
 H      -5.573500    -2.918381    -0.834917      31.09
 H      -5.598271    -3.173824     0.724852      25.98
55
name = lig-etoh-frame_347
 C       2.792314     2.398047    -2.179487      21.67
 H       1.980876     3.070843    -2.499327      15.38
 C       3.767164     1.647651    -0.144155      36.02
 H       3.871412     1.839376     0.871741      19.19
 C       4.146875     0.386745    -0.653471      13.74
 O       4.985391    -0.551671     0.133760     255.34
 C       5.670914     0.065917     1.158451     115.87
 H       5.055177     0.410577     2.077783      26.05
 H       6.339405     0.985468     1.009620      27.18
 H       6.499629    -0.625065     1.552138      25.80
 C       3.675544     0.054957    -1.901069      20.81
 O       3.889673    -1.235331    -2.317243     225.86
 H       4.474696    -1.390593    -1.555892      22.27
 C       3.082979     1.037730    -2.635261      86.19
 H       3.009421     0.732108    -3.691562      30.42
 C       3.006428     2.555458    -0.773924      60.86
 C       2.412615     3.696367    -0.135312     118.81
 H       2.685127     4.529368    -0.708513      25.17
 O       2.849415     3.900819     1.231613     341.47
 H       3.765705     4.137601     1.320153      31.99
 C       0.936504     3.803108    -0.213177      60.47
 H       0.645629     3.576941    -1.217588      19.10
 C       0.505985     5.263607     0.014790     104.88
 O       0.900412     6.124625    -1.012941     215.62
 H       0.492360     5.962533    -2.010753      25.29
 H       1.159188     5.537702     0.930054      24.00
 H      -0.631029     5.506006     0.016991      22.67
 C      -1.178579    -0.462173     0.056980      41.01
 H      -0.702447    -1.528205    -0.475831      15.61
 C      -2.972346     1.058743    -0.009835      66.56
 H      -3.930590     1.036324    -0.477531      19.51
 C      -2.198417     2.110041     0.450524      15.65
 O      -2.606940     3.373881     0.939013     205.91
 C      -4.023473     3.581032     1.190009     123.29
 H      -4.493323     2.964472     0.371908      24.84
 H      -4.160763     3.314747     2.161737      28.41
 H      -4.318892     4.690761     1.128600      26.18
 C      -0.768769     1.838871     0.404394      16.94
 O       0.260976     2.814314     0.665083     184.17
 C      -0.272080     0.561614     0.251268      41.72
 H       0.814339     0.341800     0.298231      17.29
 C      -2.510969    -0.196544    -0.248767      39.28
 C      -3.490641    -1.311017    -0.703971      66.79
 H      -4.442273    -0.873365    -1.063060      22.99
 O      -3.058694    -1.959880    -1.918359     249.20
 H      -3.522967    -2.910762    -1.734846      18.79
 C      -3.933405    -2.415739     0.497579      64.42
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 H      -3.166636    -3.173322     0.964540      19.23
 O      -4.637694    -1.597946     1.474019     272.52
 H      -3.945853    -1.365250     2.358761      21.58
 C      -4.958215    -3.354104    -0.122455      82.59
 O      -4.354744    -4.557746    -0.586668     233.78
 H      -3.701345    -4.962728     0.151510      25.42
 H      -5.592134    -3.018169    -1.069841      26.32
 H      -5.560168    -3.511119     0.862806      25.75
55
name = lig-etoh-frame_348
 C       2.730798     2.313559    -2.156525      10.44
 H       2.068290     2.932773    -2.803274      19.54
 C       3.764298     1.603336    -0.092422      59.19
 H       3.925030     1.561115     1.087360      16.02
 C       4.120345     0.402580    -0.657897      31.26
 O       4.953940    -0.536194     0.135584     234.19
 C       5.690033     0.109919     1.175764     122.59
 H       5.074795     0.416566     1.984839      29.32
 H       6.352822     0.919646     0.946904      31.29
 H       6.239568    -0.760712     1.527081      27.55
 C       3.648910     0.062995    -1.954616      16.34
 O       3.871807    -1.294227    -2.336515     132.89
 H       4.579051    -1.816213    -1.624188      20.10
 C       3.086637     1.126481    -2.660522      91.75
 H       3.227206     0.963482    -3.753697      26.48
 C       2.974192     2.530597    -0.840530      48.52
 C       2.417565     3.736661    -0.178703     113.05
 H       3.011429     4.742820    -0.869165      20.18
 O       2.814435     3.958964     1.253531     283.65
 H       3.792539     4.220101     1.335767      30.24
 C       0.929044     3.825523    -0.243959      68.89
 H       0.279219     3.580020    -1.188025      17.98
 C       0.511903     5.247043    -0.006313     121.34
 O       0.869860     6.143831    -1.039315     217.18
 H       0.282060     6.180581    -1.966504      25.69
 H       0.970564     5.738886     0.874378      26.73
 H      -0.417273     5.556558     0.381531      26.54
 C      -1.144766    -0.523173    -0.003782      48.56
 H      -0.902100    -1.398127    -0.305460      20.11
 C      -2.976831     1.049019     0.036816      52.88
 H      -4.005610     1.480571    -0.318272      20.71
 C      -2.232252     2.116223     0.540627       0.37
 O      -2.627747     3.420905     0.904909     196.52
 C      -4.055500     3.587935     1.190782     121.17
 H      -4.756655     2.996042     0.597198      26.04
 H      -4.451080     3.016044     2.263037      24.52
 H      -4.268068     4.656120     1.053117      26.53
 C      -0.719091     1.873982     0.385849      -1.97
 O       0.295312     2.830328     0.772738     142.56
 C      -0.263173     0.484109     0.300966      36.74
 H       0.769922     0.255425     0.338851      18.55
 C      -2.510300    -0.288167    -0.282127      21.81
 C      -3.527914    -1.366695    -0.720675      68.00
 H      -4.329621    -0.630339    -1.082120      21.27
 O      -3.011868    -1.988041    -1.893382     299.90
 H      -3.446170    -2.792011    -1.810983      23.92
 C      -3.928285    -2.394632     0.549065      88.29
 H      -3.121582    -2.909794     0.961935      22.41
 O      -4.599859    -1.629032     1.480595     391.26
 H      -3.899383    -1.291459     1.985774      31.48
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 C      -5.024617    -3.293763    -0.026742      99.44
 O      -4.366063    -4.575675    -0.639396     261.42
 H      -3.635668    -4.881407    -0.090547      27.63
 H      -5.487681    -3.076955    -0.946082      27.72
 H      -5.664932    -3.967592     0.593521      23.98
55
name = lig-etoh-frame_349
 C       2.632406     2.259814    -2.156296      68.05
 H       2.341586     2.904005    -2.956550      27.99
 C       3.744170     1.563634    -0.010373      29.97
 H       3.901311     1.665758     0.974405      21.28
 C       4.112310     0.391627    -0.638083      13.09
 O       4.892634    -0.499857     0.093580     205.94
 C       5.719776     0.116158     1.224603      95.58
 H       4.979306     0.477173     2.022574      25.60
 H       6.340209     0.928411     0.679209      28.16
 H       6.148021    -0.829828     1.615851      25.43
 C       3.672625     0.023722    -1.947240      24.12
 O       3.861341    -1.346264    -2.369003     219.28
 H       4.446932    -1.886530    -1.975353      27.82
 C       3.121572     1.120170    -2.775292      61.48
 H       3.145866     1.219085    -3.936643      17.07
 C       2.966689     2.502849    -0.832308      24.06
 C       2.483081     3.825618    -0.214416      98.81
 H       2.899285     4.594159    -0.733776      20.47
 O       2.773146     4.012244     1.261102     289.28
 H       3.810892     4.231924     1.152865      25.07
 C       0.832252     3.831097    -0.284321      51.26
 H       0.411392     3.513176    -1.180816      21.22
 C       0.496935     5.294948     0.028698     101.11
 O       0.846159     6.193127    -1.094760     247.39
 H       0.235095     6.060132    -1.731698      31.91
 H       1.115034     5.756970     0.857152      24.24
 H      -0.556586     5.188512     0.577899      23.40
 C      -1.157270    -0.591666    -0.092515      32.64
 H      -0.753686    -1.831545    -0.134584      16.24
 C      -3.036771     1.050551     0.059464      33.75
 H      -3.986156     1.566773     0.034157      20.86
 C      -2.144439     2.121423     0.606432     -15.14
 O      -2.662226     3.444978     0.864943     168.49
 C      -4.106946     3.538012     1.222316     114.63
 H      -4.933878     3.121389     0.540169      25.51
 H      -4.372765     3.191893     2.110770      29.45
 H      -4.268235     4.755234     1.118418      24.49
 C      -0.675611     1.909298     0.418922      -3.10
 O       0.322222     2.850614     0.879277     121.19
 C      -0.267539     0.479588     0.337799      16.19
 H       0.918343     0.346284     0.417827      16.46
 C      -2.521404    -0.337642    -0.276243      19.19
 C      -3.537093    -1.363376    -0.712238      73.92
 H      -4.437204    -0.773858    -0.882002      23.34
 O      -2.960191    -2.036791    -1.872879     254.24
 H      -3.347865    -2.991088    -2.099504      20.18
 C      -3.965187    -2.339179     0.517457      75.94
 H      -2.906457    -2.729272     0.906151      19.04
 O      -4.577676    -1.635355     1.504553     346.10
 H      -3.849520    -1.170730     2.007767      28.66
 C      -5.062119    -3.356792     0.049712      81.76
 O      -4.367589    -4.585467    -0.714504     241.07
 H      -3.539686    -4.777107    -0.157733      26.77
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 H      -5.631831    -2.763756    -0.807688      25.54
 H      -5.873588    -3.859573     0.573253      24.91
55
name = lig-etoh-frame_350
 C       2.570178     2.205915    -2.181046     107.03
 H       2.466633     3.172642    -2.800061      28.77
 C       3.669738     1.573957     0.000501      35.07
 H       3.915169     1.986257     1.098806      19.76
 C       4.103738     0.361773    -0.613283      17.28
 O       4.844070    -0.479420     0.061061     207.34
 C       5.702086     0.096484     1.243264     102.44
 H       5.102401     0.609629     1.966303      26.29
 H       6.293750     0.788626     0.746244      28.90
 H       6.304666    -0.727131     1.700881      25.60
 C       3.717675    -0.025042    -1.951992      11.66
 O       3.822128    -1.354413    -2.440556     187.21
 H       4.633146    -1.905371    -2.009081      22.79
 C       3.175352     1.034502    -2.892241      12.60
 H       3.009831     1.096530    -3.934751      19.93
 C       2.970224     2.487786    -0.749928      14.23
 C       2.480525     3.838345    -0.200876      76.37
 H       2.901283     4.919122    -0.904142      19.22
 O       2.758956     4.064168     1.226621     340.19
 H       3.678079     4.209996     1.258404      29.73
 C       0.790144     3.844192    -0.277974      22.71
 H       0.558011     3.373284    -1.332725      16.81
 C       0.455649     5.353803     0.107800      99.82
 O       0.809790     6.240367    -1.121752     138.85
 H       0.056340     5.804886    -1.881716      22.91
 H       1.326969     5.527594     0.815669      23.42
 H      -0.537220     5.117722     0.336611      23.66
 C      -1.137504    -0.671687    -0.160694      34.23
 H      -0.783930    -1.557045     0.014422      20.45
 C      -3.026158     1.061030     0.111948      33.34
 H      -4.151000     1.207952     0.189413      20.49
 C      -2.040837     2.100141     0.610071      -9.90
 O      -2.703922     3.434069     0.825619     139.02
 C      -4.154581     3.539140     1.207214     108.69
 H      -4.755853     3.218807     0.392732      26.09
 H      -4.225137     3.260376     2.463239      23.25
 H      -4.294613     4.558984     1.309278      27.48
 C      -0.648614     1.905856     0.512526       8.68
 O       0.337720     2.881595     0.944711     127.62
 C      -0.272197     0.514046     0.338061      12.40
 H       0.722699     0.461966     0.485549      18.61
 C      -2.563591    -0.305009    -0.242934       5.73
 C      -3.551885    -1.368646    -0.695825      71.43
 H      -4.639000    -1.035493    -0.907043      22.25
 O      -2.912552    -2.095221    -1.854798     237.00
 H      -3.332910    -2.982171    -2.210610      21.27
 C      -3.964034    -2.317706     0.457673      92.11
 H      -3.058582    -2.746358     0.731197      23.24
 O      -4.579908    -1.607948     1.551487     288.09
 H      -3.880204    -1.069489     2.231574      24.79
 C      -5.075154    -3.456660     0.032666      76.31
 O      -4.377704    -4.562449    -0.778729     261.97
 H      -3.562857    -4.692672    -0.162104      26.79
 H      -5.648775    -2.686969    -0.459947      27.42
 H      -5.863838    -3.560878     0.913269      25.86
55
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name = lig-etoh-frame_351
 C       2.605429     2.153759    -2.197894      89.28
 H       2.387323     3.131487    -2.543979      25.74
 C       3.597964     1.603597     0.015770      52.84
 H       3.959801     2.014613     0.903848      22.38
 C       4.056441     0.375053    -0.613547       6.20
 O       4.849399    -0.512543     0.090589     215.16
 C       5.659337     0.057530     1.223156     108.77
 H       5.120290     0.684820     1.994029      24.95
 H       6.424336     0.843046     0.812841      26.38
 H       6.334352    -0.654241     1.668155      25.91
 C       3.744105    -0.040254    -2.006838      15.13
 O       3.797868    -1.355326    -2.508483     181.42
 H       4.719561    -1.684747    -2.072586      22.35
 C       3.197555     0.966937    -2.891037      22.04
 H       2.906737     0.630630    -4.034073      19.09
 C       2.930613     2.496753    -0.738915      13.85
 C       2.436290     3.845100    -0.190091     100.07
 H       2.653058     4.630747    -0.813457      23.23
 O       2.747924     4.112830     1.174326     319.90
 H       3.783261     4.256361     1.442990      26.26
 C       0.834639     3.851334    -0.248648      38.73
 H       0.531718     3.420370    -1.154669      19.27
 C       0.449258     5.363165     0.124061      91.38
 O       0.719231     6.252353    -1.128756     224.45
 H       0.416393     5.838520    -1.949841      28.71
 H       1.127622     5.525750     0.937353      24.55
 H      -0.716563     5.548031     0.270780      22.72
 C      -1.134004    -0.588061    -0.171335      30.91
 H      -0.723402    -1.773993     0.022764      17.98
 C      -2.957348     1.043329     0.181703      54.68
 H      -4.040839     0.843203     0.282297      19.15
 C      -2.058931     2.090576     0.569047       1.06
 O      -2.719885     3.401568     0.790457     166.70
 C      -4.140987     3.533390     1.239891     103.45
 H      -4.733595     3.086458     0.356899      24.41
 H      -4.260754     3.103561     2.113062      29.03
 H      -4.329558     4.761750     1.439911      24.02
 C      -0.628603     1.881288     0.633353      12.75
 O       0.335599     2.915676     0.959412     146.15
 C      -0.316405     0.531340     0.296040      24.53
 H       0.858263     0.349729     0.553279      16.32
 C      -2.586497    -0.240598    -0.207945      11.23
 C      -3.604384    -1.395828    -0.699300      76.45
 H      -4.508424    -1.048233    -1.187987      23.12
 O      -2.868241    -2.140792    -1.829964     263.50
 H      -3.452197    -2.816916    -2.006293      25.61
 C      -3.955086    -2.340124     0.429467      77.26
 H      -3.039708    -3.009228     0.775419      19.27
 O      -4.594683    -1.562764     1.593463     327.51
 H      -3.977003    -1.366133     2.222108      30.14
 C      -5.058304    -3.492895     0.024047      82.85
 O      -4.411744    -4.506853    -0.807670     291.91
 H      -3.684197    -4.753819    -0.255085      31.32
 H      -5.833886    -2.943374    -0.631500      27.73
 H      -5.352224    -3.675129     1.057306      27.82
55
name = lig-etoh-frame_352
 C       2.707632     2.114244    -2.173999      80.12
 H       2.117471     2.927304    -2.783815      23.18
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 C       3.569055     1.587320     0.004041      51.76
 H       4.066739     1.884371     0.993327      20.70
 C       4.003303     0.396235    -0.629694       3.95
 O       4.878518    -0.560117     0.153598     226.73
 C       5.633711     0.057219     1.176319     116.30
 H       5.016092     0.495288     1.981478      25.42
 H       6.315903     0.799837     0.844641      28.26
 H       6.193235    -0.829886     1.639367      24.78
 C       3.740392    -0.014157    -2.050652      20.74
 O       3.813832    -1.340215    -2.555429     212.23
 H       4.578877    -1.690436    -2.252184      26.33
 C       3.159991     0.919289    -2.840648      44.23
 H       2.952230     0.435204    -3.694684      21.27
 C       2.848837     2.505014    -0.828826      47.11
 C       2.351476     3.789041    -0.163830      93.85
 H       2.674710     4.802005    -1.078546      18.72
 O       2.757874     4.163205     1.146414     305.23
 H       3.738920     4.282632     1.243141      27.24
 C       0.883856     3.868211    -0.157738      51.91
 H       0.343025     3.499610    -1.110573      17.23
 C       0.403284     5.349613     0.063065     103.12
 O       0.649118     6.259547    -1.096344     219.68
 H       0.574974     5.765894    -2.044908      24.80
 H       0.831476     5.845667     1.061914      23.75
 H      -0.512237     5.761508     0.329828      24.62
 C      -1.154236    -0.466355    -0.124564      51.99
 H      -0.873163    -1.455809    -0.306354      19.18
 C      -2.905157     0.989312     0.252221      54.74
 H      -3.984833     1.094914     0.431098      19.80
 C      -2.143482     2.122194     0.534039       6.23
 O      -2.702800     3.363976     0.764605     206.22
 C      -4.094344     3.547032     1.222621     116.23
 H      -4.816629     3.110472     0.568005      26.02
 H      -4.429786     2.650784     2.138415      22.39
 H      -4.259960     4.496578     1.354581      28.18
 C      -0.650037     1.873403     0.725028      -1.80
 O       0.317582     2.938222     0.945168     170.93
 C      -0.295162     0.521811     0.262010      50.26
 H       0.646723     0.203294     0.420386      20.38
 C      -2.541309    -0.239310    -0.201099      11.41
 C      -3.601451    -1.398974    -0.719595      69.84
 H      -4.374280    -0.862586    -1.367213      21.01
 O      -2.834386    -2.167371    -1.777247     220.94
 H      -3.638834    -2.869897    -1.879820      20.43
 C      -3.971513    -2.391466     0.440002      80.47
 H      -3.162585    -2.960765     0.820974      20.61
 O      -4.617894    -1.541034     1.582751     269.43
 H      -3.840240    -1.762784     2.407750      19.89
 C      -5.015921    -3.454480     0.018279      95.92
 O      -4.454885    -4.449413    -0.824722     245.34
 H      -3.692430    -4.959164    -0.348706      27.73
 H      -5.963967    -3.474736    -0.580735      25.33
 H      -5.015489    -4.118329     0.999099      26.59
55
name = lig-etoh-frame_353
 C       2.763068     2.138533    -2.205095      61.55
 H       2.068842     2.419963    -2.957650      17.05
 C       3.572169     1.554836    -0.046444      55.54
 H       3.926111     1.688120     1.011382      18.04
 C       3.995536     0.367491    -0.634492       9.14
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 O       4.875268    -0.589026     0.174049     221.47
 C       5.614324     0.028382     1.167700     113.37
 H       4.900244     0.314301     1.991717      25.48
 H       6.287221     0.875653     0.775386      26.99
 H       6.066983    -0.838763     1.586237      26.13
 C       3.749848    -0.016434    -2.003603      15.65
 O       3.833097    -1.299311    -2.596154     141.35
 H       4.688055    -1.959008    -2.298273      20.37
 C       3.097418     0.905012    -2.745761      77.94
 H       2.773623     0.484709    -3.865552      23.09
 C       2.800779     2.478490    -0.888790      75.34
 C       2.298907     3.785930    -0.210257     122.50
 H       2.566523     4.446111    -0.836354      30.01
 O       2.782786     4.202407     1.121979     295.38
 H       3.757222     4.302856     0.983645      30.13
 C       0.822616     3.883150    -0.069159      69.76
 H       0.354818     3.642475    -1.027071      22.97
 C       0.362956     5.385991     0.027282     108.99
 O       0.600142     6.263378    -1.063912     240.46
 H       0.626279     5.656313    -1.990135      26.49
 H       0.840074     5.956767     0.750686      25.46
 H      -0.794699     5.401210     0.327912      24.21
 C      -1.203447    -0.367665    -0.099608      45.57
 H      -0.780856    -1.385022    -0.644580      17.37
 C      -2.947233     0.970203     0.328406      50.67
 H      -3.950006     1.446833     0.461353      18.98
 C      -2.155966     2.140702     0.529796       9.39
 O      -2.686802     3.344358     0.749914     222.62
 C      -4.048672     3.437185     1.220890     110.28
 H      -4.903740     3.266125     0.440201      24.70
 H      -4.255863     2.875497     1.978477      28.64
 H      -4.224696     4.670591     1.487989      23.63
 C      -0.712689     1.885852     0.739380      -0.85
 O       0.287017     2.944449     0.937158     192.35
 C      -0.247392     0.572872     0.268585      40.19
 H       0.836668     0.160982     0.271287      17.37
 C      -2.508980    -0.292500    -0.208667      36.17
 C      -3.514916    -1.358856    -0.737209      85.13
 H      -4.331164    -0.780839    -1.163857      23.46
 O      -2.839220    -2.199818    -1.704213     273.80
 H      -3.374137    -3.008419    -1.984791      22.44
 C      -4.059603    -2.370198     0.447340      77.16
 H      -3.086088    -2.859347     0.843437      20.43
 O      -4.590153    -1.550794     1.567673     314.90
 H      -4.249406    -2.086865     2.329443      25.25
 C      -4.975413    -3.487907     0.071523     117.46
 O      -4.456357    -4.427324    -0.885803     295.53
 H      -3.774292    -5.010669    -0.460781      29.83
 H      -6.074862    -3.440016    -0.140048      27.50
 H      -5.136539    -4.165320     0.854060      29.38
55
name = lig-etoh-frame_354
 C       2.745476     2.169790    -2.299945      38.21
 H       1.950785     2.534386    -3.030934      17.25
 C       3.566906     1.524535    -0.124090      57.60
 H       3.648433     1.687382     0.937670      20.38
 C       4.048996     0.283246    -0.615142      23.13
 O       4.826723    -0.602490     0.125782     247.67
 C       5.590055    -0.004122     1.200826     109.37
 H       4.925614     0.339793     2.022452      25.93
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 H       6.172520     0.854796     0.867144      27.27
 H       6.301056    -0.810613     1.622538      25.40
 C       3.770888    -0.076385    -1.919502      24.69
 O       3.878722    -1.269291    -2.626714     219.97
 H       4.538838    -1.904691    -2.258124      24.32
 C       3.034583     0.869722    -2.704225      62.09
 H       2.706538     0.853214    -3.644833      28.63
 C       2.806403     2.439533    -0.850663      57.25
 C       2.247669     3.749123    -0.227615      81.52
 H       2.633571     4.756925    -1.134390      21.98
 O       2.825036     4.220423     1.085774     222.39
 H       3.883470     4.355611     0.890948      27.38
 C       0.700504     3.898045    -0.030804      68.55
 H       0.353039     3.607471    -1.081788      21.41
 C       0.265808     5.428562     0.047943     113.93
 O       0.565107     6.247789    -1.072174     272.80
 H       0.460968     5.794293    -1.850413      34.50
 H       0.980759     5.956629     0.840221      23.32
 H      -0.703026     4.949607     0.144090      23.19
 C      -1.149888    -0.371103    -0.127502      34.16
 H      -0.633455    -1.066294    -0.815441      18.67
 C      -3.033932     1.001156     0.384650      51.45
 H      -4.079920     1.261182     0.310615      18.72
 C      -2.103237     2.078756     0.553749      13.80
 O      -2.679005     3.358005     0.742905     203.02
 C      -4.030138     3.410639     1.179667     109.64
 H      -4.672780     3.388468     0.338204      26.05
 H      -4.140269     2.775542     2.328419      22.05
 H      -4.067585     4.300180     1.607074      27.97
 C      -0.740835     1.911479     0.676139      14.81
 O       0.242524     2.943825     0.951661     208.19
 C      -0.204543     0.666736     0.311968      28.97
 H       0.885272     0.546155     0.090094      17.85
 C      -2.578511    -0.292928    -0.179337      27.92
 C      -3.435491    -1.338739    -0.721672      90.24
 H      -4.382964    -0.783164    -1.030274      22.53
 O      -2.832011    -2.228687    -1.647341     310.02
 H      -3.224295    -3.021955    -1.888212      25.58
 C      -4.101776    -2.294430     0.465061      95.48
 H      -3.115935    -2.692252     0.735569      23.72
 O      -4.578713    -1.584779     1.533307     326.08
 H      -4.497359    -2.092238     2.352247      27.77
 C      -4.988418    -3.575944     0.143866      78.13
 O      -4.444190    -4.418967    -0.987160     295.26
 H      -3.823084    -4.919751    -0.469711      30.21
 H      -5.988656    -2.971009     0.096397      27.06
 H      -5.187316    -4.120318     1.195703      28.67
55
name = lig-etoh-frame_355
 C       2.662114     2.193997    -2.346832      17.20
 H       2.092873     2.992092    -2.848939      13.64
 C       3.559321     1.491379    -0.173384      50.88
 H       3.404022     1.757629     0.968008      18.59
 C       4.117617     0.216115    -0.602036      31.73
 O       4.792632    -0.625578     0.086390     242.05
 C       5.571948    -0.049224     1.257230     107.69
 H       4.966464     0.338307     2.080385      26.19
 H       6.095042     0.884571     0.905842      26.83
 H       6.379992    -0.666507     1.547062      27.00
 C       3.745561    -0.130937    -1.901103      30.21
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 O       3.934790    -1.255482    -2.648037     227.48
 H       4.505807    -1.834760    -2.140682      25.43
 C       2.997044     0.861009    -2.654172      55.17
 H       2.689698     0.739542    -3.830457      25.54
 C       2.824910     2.428803    -0.844478      45.25
 C       2.236049     3.777391    -0.264351     104.70
 H       2.356750     4.420508    -0.915960      27.69
 O       2.882475     4.219168     1.026246     309.90
 H       3.789860     4.356429     1.019056      33.01
 C       0.637475     3.894447    -0.080293      58.18
 H       0.231119     3.501920    -1.047353      18.85
 C       0.194254     5.422182     0.105929     103.53
 O       0.534749     6.238875    -1.077956     239.02
 H       0.104951     5.797756    -2.078864      21.15
 H       0.579335     5.741437     1.019268      26.35
 H      -0.946067     5.244709     0.176369      23.00
 C      -1.055613    -0.358048    -0.179645      39.01
 H      -0.513299    -1.085483    -0.872875      17.92
 C      -3.104019     0.999376     0.387035      50.42
 H      -4.207428     0.990144     0.224194      19.93
 C      -2.126642     2.022075     0.603572       5.66
 O      -2.641479     3.368063     0.736828     199.08
 C      -3.996145     3.378228     1.204245     105.72
 H      -4.692785     3.277527     0.298154      25.37
 H      -4.185626     2.685032     1.889547      29.25
 H      -4.039494     4.489707     1.786376      23.94
 C      -0.701775     1.952633     0.590744      27.08
 O       0.178764     2.952653     0.982790     206.70
 C      -0.209473     0.731868     0.323283      26.96
 H       0.841717     0.872582     0.053444      18.04
 C      -2.588281    -0.218155    -0.097959      27.31
 C      -3.470453    -1.352740    -0.681335      78.34
 H      -4.316343    -0.879195    -1.219463      22.79
 O      -2.787364    -2.226814    -1.611449     230.58
 H      -3.449304    -3.146227    -1.568239      15.26
 C      -4.035105    -2.267314     0.471849      97.38
 H      -3.042413    -2.722617     0.781950      20.31
 O      -4.610093    -1.587666     1.501067     265.33
 H      -4.560593    -2.044718     2.509782      25.20
 C      -5.031031    -3.601890     0.231317      82.11
 O      -4.456117    -4.400096    -1.058934     225.80
 H      -3.735926    -4.890379    -0.480408      25.09
 H      -5.822624    -2.981248    -0.113359      28.02
 H      -4.980092    -4.075740     1.154855      31.20
55
name = lig-etoh-frame_356
 C       2.573284     2.209926    -2.276125      55.02
 H       2.374357     3.164241    -2.821813      21.13
 C       3.543922     1.457617    -0.140616      42.36
 H       3.510638     1.622857     0.866578      20.26
 C       4.115449     0.242026    -0.650210      14.44
 O       4.825208    -0.692823     0.127038     221.71
 C       5.556884    -0.062855     1.282281     100.66
 H       4.880773     0.133051     2.191826      24.84
 H       5.951855     0.899927     0.864744      26.96
 H       6.378933    -0.807173     1.517112      24.61
 C       3.666886    -0.119965    -1.938768      16.00
 O       4.005320    -1.266685    -2.665961     170.35
 H       4.581226    -1.919977    -1.956153      22.39
 C       2.944055     0.886890    -2.692119      52.45
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 H       2.907721     0.333670    -3.583333      20.21
 C       2.828376     2.448649    -0.922644      29.96
 C       2.232147     3.759396    -0.239515      75.75
 H       2.322849     4.710296    -1.299438      17.29
 O       2.899598     4.205351     0.964950     241.15
 H       3.952904     4.324586     0.994796      26.23
 C       0.618736     3.871940    -0.144251      51.76
 H       0.102498     3.480397    -1.028933      18.59
 C       0.073802     5.354289     0.124218      96.98
 O       0.496459     6.219545    -1.089982     238.31
 H      -0.005299     5.883385    -1.763806      31.42
 H       0.334861     5.765899     1.176294      24.76
 H      -0.915499     5.729729     0.199832      24.66
 C      -1.004392    -0.299148    -0.223065      51.95
 H      -0.574025    -1.288339    -0.743531      18.50
 C      -3.134144     0.965702     0.355991      48.49
 H      -4.218153     1.032541     0.340155      20.99
 C      -2.206235     2.038742     0.658731      -1.87
 O      -2.590152     3.356905     0.741282     198.09
 C      -3.962997     3.424426     1.212425     112.05
 H      -4.729072     3.261984     0.465115      27.31
 H      -4.318006     2.283596     1.812313      23.21
 H      -4.199585     4.301869     1.666452      27.75
 C      -0.716759     2.003539     0.538736      22.50
 O       0.109651     2.990706     1.010575     185.97
 C      -0.213573     0.723515     0.262918      29.12
 H       0.948173     0.848154     0.099873      16.88
 C      -2.485691    -0.179967    -0.035846      23.32
 C      -3.538296    -1.359356    -0.640493      71.97
 H      -4.267047    -0.933302    -1.380191      20.98
 O      -2.759585    -2.245649    -1.572062     269.31
 H      -3.313812    -2.932052    -1.391545      23.81
 C      -3.908816    -2.322481     0.488383      88.64
 H      -2.998537    -2.810940     0.937150      19.01
 O      -4.681436    -1.555720     1.506758     320.94
 H      -4.351889    -1.900112     2.308738      28.79
 C      -5.008397    -3.539528     0.231775      72.82
 O      -4.474695    -4.378095    -1.066716     236.49
 H      -3.689686    -4.864592    -0.744079      28.14
 H      -6.043028    -3.342149    -0.319165      25.25
 H      -4.923528    -4.282787     1.136934      26.87
55
name = lig-etoh-frame_357
 C       2.513620     2.201764    -2.212359      72.61
 H       2.470058     2.963876    -2.987578      25.83
 C       3.516053     1.438806    -0.116971      47.13
 H       3.786132     1.536080     1.058094      18.17
 C       4.075008     0.285436    -0.693303     -12.23
 O       4.869124    -0.749578     0.181872     193.21
 C       5.534778    -0.088838     1.288186     117.49
 H       4.879433    -0.111863     2.142374      26.83
 H       5.892503     0.880989     0.976885      28.02
 H       6.269166    -0.843428     1.528551      25.86
 C       3.582632    -0.066846    -1.986672      11.51
 O       4.086937    -1.291715    -2.653448     207.13
 H       4.534844    -1.831636    -2.063627      27.04
 C       2.907916     0.888038    -2.744563      47.68
 H       2.865191     0.292266    -3.745939      18.38
 C       2.831082     2.469492    -0.940556      28.51
 C       2.244408     3.794579    -0.299025     102.01
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 H       2.354958     4.442923    -0.953016      25.24
 O       2.898826     4.187862     0.912402     281.57
 H       3.914117     4.190247     0.749849      27.81
 C       0.597643     3.856473    -0.157178      38.89
 H       0.119637     3.463892    -1.144795      19.47
 C      -0.013685     5.307139     0.117399      95.36
 O       0.475622     6.205174    -1.046681     182.07
 H      -0.153972     5.823703    -1.826227      24.76
 H       0.508157     5.782335     0.954001      24.69
 H      -1.120678     5.620532    -0.009548      22.64
 C      -1.027540    -0.276746    -0.254173      60.06
 H      -0.729895    -1.239791    -0.520487      21.16
 C      -3.100979     0.965868     0.337558      51.76
 H      -4.170064     1.113467     0.480538      20.79
 C      -2.240287     2.079928     0.676224       8.85
 O      -2.581475     3.359419     0.773124     212.85
 C      -3.967598     3.400195     1.220382     117.87
 H      -4.690978     3.400649     0.331762      26.11
 H      -4.143537     2.619923     1.798173      29.39
 H      -4.299835     4.393718     1.832437      24.99
 C      -0.811283     1.992945     0.530605       9.00
 O       0.042518     3.052317     1.016297     183.04
 C      -0.163434     0.742386     0.165890      34.21
 H       0.851428     0.515224     0.182330      18.86
 C      -2.379009    -0.223945    -0.040398      39.54
 C      -3.513732    -1.355464    -0.607853      68.24
 H      -4.370302    -0.897507    -1.181427      22.19
 O      -2.726632    -2.243664    -1.525871     208.02
 H      -3.234557    -3.231344    -1.538378      16.69
 C      -3.873017    -2.386501     0.534919      91.73
 H      -2.985407    -2.802520     1.001771      20.51
 O      -4.741428    -1.523221     1.508408     306.40
 H      -4.118755    -1.694266     2.340152      24.77
 C      -4.934326    -3.495783     0.157112     109.13
 O      -4.493546    -4.350417    -1.047757     262.27
 H      -3.691011    -4.858612    -0.901300      30.59
 H      -5.973068    -3.533196    -0.027972      27.51
 H      -5.058475    -4.249769     0.900237      27.68
55
name = lig-etoh-frame_358
 C       2.497869     2.131017    -2.250441      63.96
 H       2.194019     2.809190    -3.073079      23.17
 C       3.501232     1.446232    -0.074973      57.70
 H       3.849181     1.642846     0.846456      22.88
 C       4.021087     0.290757    -0.690701     -10.34
 O       4.879932    -0.759505     0.181323     177.39
 C       5.505987    -0.151038     1.290320     110.67
 H       4.789053    -0.170381     2.206380      24.76
 H       5.949808     0.930485     1.225992      25.77
 H       6.386938    -0.789310     1.582786      25.25
 C       3.562647    -0.060921    -2.024522      14.63
 O       4.136873    -1.275208    -2.640705     178.61
 H       4.652775    -1.827803    -1.946729      23.33
 C       2.873609     0.858218    -2.815092      35.38
 H       2.575007     0.870127    -3.896260      18.60
 C       2.829009     2.481536    -0.843271      29.44
 C       2.231506     3.783460    -0.334632      77.07
 H       2.530745     4.825450    -1.239991      18.82
 O       2.891278     4.164125     0.868236     295.95
 H       3.778629     4.129625     0.658022      29.49
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 C       0.558735     3.845168    -0.143535      56.29
 H       0.285760     3.470792    -1.094990      21.93
 C      -0.049948     5.296474     0.047127     103.40
 O       0.440212     6.178174    -0.993138     223.16
 H       0.070231     5.910211    -2.001559      24.83
 H       0.553730     5.725235     0.870638      23.65
 H      -1.121795     4.991844     0.026875      23.50
 C      -1.055521    -0.278763    -0.273581      36.86
 H      -0.629184    -1.451764    -0.421873      19.11
 C      -3.005125     0.985238     0.340345      62.87
 H      -4.100419     0.993472     0.519905      21.73
 C      -2.218342     2.078704     0.637450      15.09
 O      -2.624866     3.404411     0.835789     203.70
 C      -4.003673     3.451487     1.205729     107.57
 H      -4.518371     3.515471     0.252948      25.50
 H      -4.161527     2.521082     2.154057      22.56
 H      -4.079328     4.303878     1.876795      25.90
 C      -0.845316     1.932630     0.551843      10.41
 O      -0.031979     3.106347     0.987022     170.03
 C      -0.156552     0.799572     0.067742      50.20
 H       0.913713     0.328160     0.287725      17.36
 C      -2.416988    -0.269225    -0.087374      41.40
 C      -3.399662    -1.394284    -0.557282      72.36
 H      -4.369619    -0.883382    -0.818766      22.02
 O      -2.700896    -2.249327    -1.485508     272.13
 H      -3.087560    -3.102629    -1.822363      20.53
 C      -3.943420    -2.386128     0.576943      86.49
 H      -2.970717    -2.786927     1.079308      19.91
 O      -4.761406    -1.529227     1.523733     307.28
 H      -4.107032    -1.198115     2.326489      24.00
 C      -4.827088    -3.519005     0.069078      98.64
 O      -4.513841    -4.312593    -1.039909     281.24
 H      -3.697291    -4.894272    -0.770302      28.47
 H      -5.958052    -3.084186     0.097352      26.32
 H      -4.911607    -4.225678     0.999755      26.42
55
name = lig-etoh-frame_359
 C       2.515995     2.047289    -2.272869      43.54
 H       1.799146     2.733588    -2.805575      17.18
 C       3.493866     1.483434    -0.066635      48.61
 H       3.885483     1.872776     0.993015      18.80
 C       3.958348     0.257763    -0.669267       1.67
 O       4.857473    -0.722374     0.116798     220.58
 C       5.489877    -0.208133     1.346018     122.88
 H       4.812136    -0.167219     2.154299      27.48
 H       5.845134     0.785057     1.302528      28.15
 H       6.419864    -0.739117     1.570038      26.90
 C       3.617734    -0.120456    -2.053607       9.47
 O       4.162424    -1.234561    -2.619247     150.04
 H       4.784371    -1.689400    -1.826055      19.79
 C       2.819446     0.872818    -2.884310      57.31
 H       2.462742     1.080065    -3.885590      24.76
 C       2.791164     2.455196    -0.807016      38.18
 C       2.217327     3.822258    -0.385830     105.74
 H       2.380380     4.486995    -1.087878      28.94
 O       2.863707     4.142899     0.843937     265.39
 H       3.938810     4.154062     0.728274      27.23
 C       0.562774     3.844414    -0.131575      60.02
 H       0.253240     3.356777    -1.174364      20.70
 C      -0.033587     5.250768    -0.052103     117.48
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 O       0.394226     6.166493    -0.973097     325.15
 H       0.319452     5.913341    -1.840575      32.99
 H       0.194465     5.642161     1.020939      24.87
 H      -1.006034     4.750928     0.213770      23.29
 C      -1.037309    -0.340540    -0.283266      32.50
 H      -0.603121    -1.181318    -0.471357      20.26
 C      -2.940142     0.961257     0.343622      65.26
 H      -4.001298     0.922915     0.462788      20.87
 C      -2.177958     2.095901     0.577089      11.49
 O      -2.667920     3.433640     0.910870     205.37
 C      -4.027177     3.484706     1.248463     125.19
 H      -4.669308     3.498860     0.327713      26.41
 H      -4.384517     2.761533     1.848298      28.56
 H      -4.020923     4.492364     1.844184      25.24
 C      -0.767075     1.910361     0.578070       6.70
 O      -0.107297     3.131841     0.937125     198.74
 C      -0.193184     0.797282    -0.006608      59.72
 H       0.801725     0.696083     0.230840      20.16
 C      -2.505477    -0.279046    -0.147593      20.10
 C      -3.299519    -1.464460    -0.470548      87.13
 H      -4.254222    -0.922938    -0.774840      21.47
 O      -2.649257    -2.235745    -1.476892     301.62
 H      -3.257455    -2.872987    -1.827286      23.06
 C      -3.967449    -2.327989     0.634491     102.51
 H      -3.186502    -2.749088     1.176532      22.96
 O      -4.763771    -1.544906     1.536494     397.71
 H      -4.260075    -1.098143     2.094917      35.08
 C      -4.797198    -3.535982     0.077106     104.64
 O      -4.513339    -4.288460    -1.059219     343.39
 H      -3.874085    -4.854286    -0.612109      30.58
 H      -5.545155    -2.817084    -0.113829      29.02
 H      -4.724506    -4.091483     0.994148      28.64
55
name = lig-etoh-frame_360
 C       2.498491     2.032168    -2.203413      51.21
 H       1.636824     2.608332    -2.505795      17.63
 C       3.508321     1.541642    -0.051451      49.22
 H       3.770458     1.843091     0.924312      19.27
 C       3.902322     0.217547    -0.643478       0.33
 O       4.817490    -0.656768     0.025213     189.02
 C       5.474710    -0.253407     1.387734      89.13
 H       4.697892    -0.327113     2.269623      24.75
 H       5.750587     0.873516     1.175232      23.99
 H       6.338253    -0.922989     1.524483      25.73
 C       3.666195    -0.125550    -2.068854       3.49
 O       4.199312    -1.212719    -2.585648     209.39
 H       4.775174    -1.532347    -1.999384      25.73
 C       2.804422     0.866240    -2.907612      59.31
 H       2.519861     0.656569    -4.038708      24.54
 C       2.729163     2.385681    -0.875153      60.33
 C       2.188233     3.780046    -0.356140      84.97
 H       2.277172     4.605402    -1.468258      22.76
 O       2.850184     4.140040     0.842206     260.94
 H       3.827755     4.248695     0.881800      28.65
 C       0.617361     3.819174    -0.185815      75.17
 H       0.181518     3.388805    -1.022745      23.45
 C      -0.023317     5.154603    -0.061124     112.54
 O       0.347635     6.195771    -0.959690     232.02
 H       0.462225     5.667060    -2.006089      23.03
 H      -0.023392     5.579342     0.936763      24.60
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 H      -1.178386     5.126995    -0.057090      23.65
 C      -1.047545    -0.361758    -0.281665      42.05
 H      -0.392368    -1.360705    -0.742176      17.19
 C      -2.946809     0.925603     0.337398      58.77
 H      -4.062940     1.074125     0.425033      19.62
 C      -2.132141     2.131318     0.536756      -1.28
 O      -2.679712     3.407926     0.976268     183.61
 C      -4.066905     3.575509     1.273382     108.59
 H      -4.840149     3.538508     0.474320      26.10
 H      -4.682800     2.583485     1.951088      22.21
 H      -4.223484     4.631002     1.682966      25.45
 C      -0.709399     1.963101     0.582232      11.82
 O      -0.146875     3.133239     0.890853     197.25
 C      -0.251333     0.760741    -0.042598      41.20
 H       0.933242     0.941698    -0.043815      16.49
 C      -2.460313    -0.266382    -0.188050      30.85
 C      -3.276688    -1.507458    -0.397643      86.90
 H      -4.160476    -1.082721    -1.045515      19.20
 O      -2.584886    -2.228704    -1.482226     238.20
 H      -3.551360    -2.666120    -1.770876      17.71
 C      -3.891181    -2.276148     0.702736     100.38
 H      -3.147164    -2.801230     1.464233      18.67
 O      -4.803775    -1.573119     1.514603     323.81
 H      -4.121088    -1.020684     2.149118      24.99
 C      -4.805591    -3.465379     0.142647      78.33
 O      -4.486701    -4.281925    -1.086121     276.01
 H      -3.919445    -4.995133    -0.726023      28.67
 H      -5.738280    -2.904670    -0.379816      26.16
 H      -4.970023    -4.170183     1.023761      25.89
55
name = lig-etoh-frame_361
 C       2.412226     2.023273    -2.163254      60.64
 H       1.582093     2.606769    -2.625224      20.01
 C       3.523089     1.542739    -0.087173      71.22
 H       3.712897     1.775219     1.012863      19.34
 C       3.860735     0.232877    -0.615576      15.09
 O       4.781410    -0.596754    -0.049489     177.24
 C       5.419244    -0.270152     1.383079     106.11
 H       4.755762    -0.487841     2.151292      28.38
 H       5.734401     0.697118     1.267621      27.80
 H       6.177804    -1.074099     1.430457      26.55
 C       3.656192    -0.024426    -2.058039       2.57
 O       4.234456    -1.217104    -2.583928     160.62
 H       5.040873    -1.626397    -1.961689      20.83
 C       2.850924     0.793355    -2.881599      52.25
 H       2.661360     0.308315    -3.778717      24.35
 C       2.693004     2.329552    -0.909210      61.63
 C       2.167780     3.716651    -0.366778     113.02
 H       2.262192     4.420251    -1.165505      26.07
 O       2.818183     4.154723     0.861290     291.71
 H       3.772106     4.300885     0.818614      30.46
 C       0.666799     3.785729    -0.244122      60.22
 H       0.174735     3.314867    -1.220588      20.09
 C      -0.083695     5.116926    -0.049161      99.38
 O       0.331014     6.218547    -0.992841     266.34
 H       0.346022     5.765063    -1.777708      32.91
 H       0.115485     5.563572     1.008869      23.07
 H      -1.072992     5.201017    -0.544093      21.24
 C      -1.008514    -0.399584    -0.315382      52.11
 H      -0.649468    -1.150430    -0.815176      21.50
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 C      -2.984293     0.956622     0.324066      58.71
 H      -4.027420     1.162082     0.379400      19.12
 C      -2.142279     2.125830     0.534294       6.61
 O      -2.684656     3.355278     1.032313     175.13
 C      -4.166568     3.619418     1.306424     117.37
 H      -4.756423     3.597338     0.355975      26.15
 H      -4.467368     2.974235     2.004151      27.94
 H      -4.316866     4.619782     1.725320      26.88
 C      -0.751908     2.002316     0.536984      16.26
 O      -0.112670     3.141680     0.868763     206.71
 C      -0.238705     0.768046    -0.029614      38.17
 H       0.716092     0.729157    -0.531028      19.05
 C      -2.366965    -0.262591    -0.180518      29.63
 C      -3.277752    -1.472533    -0.406908      88.22
 H      -4.126971    -1.256260    -1.043121      21.08
 O      -2.553636    -2.248349    -1.483142     280.78
 H      -3.257608    -2.731592    -1.913144      22.87
 C      -3.794711    -2.321940     0.792103      93.40
 H      -3.074489    -2.726259     1.393522      25.04
 O      -4.841067    -1.566366     1.497320     333.47
 H      -4.267720    -1.166397     2.281543      26.82
 C      -4.855750    -3.379848     0.182656      99.25
 O      -4.445286    -4.274346    -1.090559     230.77
 H      -3.884862    -5.117489    -0.933617      28.01
 H      -5.797109    -3.154042    -0.180677      28.25
 H      -5.384256    -4.093292     0.853480      25.32
55
name = lig-etoh-frame_362
 C       2.278628     1.959994    -2.250815      57.03
 H       1.709181     2.619768    -2.906331      20.85
 C       3.530484     1.490975    -0.123404      79.19
 H       3.646787     1.734437     0.967702      17.62
 C       3.845708     0.311408    -0.614861      38.29
 O       4.766159    -0.559103    -0.078225     199.64
 C       5.341810    -0.322472     1.304371     103.51
 H       4.558796    -0.552911     2.159039      25.95
 H       5.882814     0.742996     1.500144      24.64
 H       6.119837    -1.078662     1.320956      27.26
 C       3.667915     0.037781    -2.004202      23.12
 O       4.266946    -1.217585    -2.580359     154.35
 H       5.051250    -1.555547    -2.002244      22.38
 C       2.906192     0.741738    -2.780953      48.61
 H       2.630135     0.190613    -3.796503      20.52
 C       2.680907     2.327735    -0.861957      79.36
 C       2.161532     3.621056    -0.349047      97.98
 H       2.504509     4.617323    -1.162693      20.88
 O       2.767283     4.167003     0.891668     202.79
 H       3.802307     4.317750     0.604645      28.54
 C       0.636524     3.750604    -0.311021      73.99
 H       0.413769     3.347053    -1.232237      20.23
 C      -0.124953     5.157323    -0.076323      92.86
 O       0.347998     6.257488    -1.002605     220.79
 H       0.185567     5.812503    -2.056865      23.66
 H       0.063556     5.417237     0.903010      25.32
 H      -1.124992     4.764647    -0.498752      20.82
 C      -0.967295    -0.361064    -0.337466      26.74
 H      -0.633731    -1.346154    -1.035454      16.46
 C      -2.981882     1.004042     0.287759      50.85
 H      -4.098926     1.059296     0.336041      21.11
 C      -2.236583     2.095065     0.578652      17.53
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 O      -2.699462     3.313864     1.085965     158.11
 C      -4.221609     3.654956     1.292366      87.82
 H      -4.624510     3.572242     0.264369      24.13
 H      -4.532272     2.917638     2.341741      21.80
 H      -4.175589     4.738978     1.826395      23.60
 C      -0.812457     1.992737     0.455073      16.63
 O      -0.025480     3.141575     0.856336     200.08
 C      -0.204294     0.786376    -0.029627      43.38
 H       0.663079     0.616810    -0.722222      17.48
 C      -2.358405    -0.253336    -0.124374      32.14
 C      -3.266022    -1.433535    -0.471845      59.93
 H      -4.318136    -1.105827    -0.836085      21.12
 O      -2.513210    -2.279150    -1.477674     239.06
 H      -3.031321    -2.976985    -1.971925      20.72
 C      -3.788098    -2.391884     0.815702      70.76
 H      -2.851664    -2.791478     1.423626      18.38
 O      -4.849820    -1.542326     1.504205     317.02
 H      -4.584806    -1.364286     2.375030      30.24
 C      -4.886888    -3.381292     0.193790      79.43
 O      -4.412048    -4.250792    -1.084836     245.61
 H      -3.867121    -4.997339    -0.814822      29.35
 H      -5.878559    -2.777688    -0.194368      26.54
 H      -5.331035    -4.060309     0.949034      26.62
55
name = lig-etoh-frame_363
 C       2.195348     1.877331    -2.315535     121.44
 H       1.832577     2.577150    -3.095043      29.04
 C       3.480355     1.510953    -0.106022      57.26
 H       3.694116     1.742398     0.895752      19.45
 C       3.907864     0.331249    -0.659155      44.34
 O       4.775250    -0.532301    -0.060727     262.65
 C       5.260418    -0.365840     1.223324     139.04
 H       4.506535    -0.511886     1.928394      28.97
 H       5.739607     0.487340     1.555862      29.36
 H       6.083075    -1.106344     1.303180      26.90
 C       3.750924    -0.034283    -1.921668      29.03
 O       4.279518    -1.184596    -2.563515     234.31
 H       4.951106    -1.450212    -2.010430      26.07
 C       2.864478     0.754274    -2.744439      33.46
 H       2.654328     0.449103    -3.693804      19.92
 C       2.648197     2.330185    -0.885701      86.39
 C       2.175748     3.622850    -0.322658     115.75
 H       2.524509     4.395605    -1.109920      22.30
 O       2.728627     4.160606     0.912213     255.52
 H       3.627457     4.294945     0.694146      33.36
 C       0.601165     3.761440    -0.344189      66.46
 H       0.338970     3.258969    -1.384115      19.35
 C      -0.127669     5.175303    -0.201238      89.93
 O       0.362256     6.270915    -1.021720     274.87
 H       0.006787     6.106308    -1.968827      26.81
 H      -0.124815     5.434856     0.972554      23.88
 H      -1.155257     4.694801    -0.080106      23.20
 C      -0.967544    -0.321253    -0.365734      44.83
 H      -0.558726    -1.160995    -0.855331      20.22
 C      -3.008903     0.979220     0.232791      73.01
 H      -4.086244     0.891474     0.322043      23.58
 C      -2.303928     2.098734     0.654768      11.44
 O      -2.735847     3.293569     1.143372     197.12
 C      -4.198584     3.653078     1.327453     126.16
 H      -4.732052     3.540976     0.385217      27.53
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 H      -4.737704     3.064774     1.989030      28.47
 H      -4.098235     4.612186     1.623182      28.24
 C      -0.835556     1.981161     0.384217       5.90
 O       0.056651     3.091465     0.825786     179.88
 C      -0.177409     0.794866    -0.072185      30.00
 H       0.896775     0.909669    -0.507906      15.47
 C      -2.388976    -0.246711    -0.072474      26.34
 C      -3.272273    -1.436831    -0.532013      54.65
 H      -4.234748    -0.923068    -0.701558      22.24
 O      -2.476279    -2.288321    -1.470686     178.09
 H      -3.038662    -3.243253    -1.641578      14.32
 C      -3.831893    -2.429403     0.778287      82.78
 H      -3.033272    -2.789114     1.369019      20.47
 O      -4.826667    -1.519305     1.508595     261.63
 H      -4.802885    -1.676059     2.622464      25.46
 C      -4.909350    -3.409851     0.166618      82.26
 O      -4.399526    -4.205226    -1.054157     274.29
 H      -3.848131    -4.807469    -0.493676      27.71
 H      -5.426517    -2.594245    -0.177047      30.45
 H      -5.081747    -4.078467     1.064015      28.15
55
name = lig-etoh-frame_364
 C       2.179646     1.845177    -2.294081      86.48
 H       1.786025     2.493058    -3.081409      26.62
 C       3.389457     1.567406    -0.097487      80.39
 H       3.816429     1.877788     0.972574      21.84
 C       4.019952     0.329060    -0.663864      41.28
 O       4.809055    -0.529096    -0.050135     262.24
 C       5.208136    -0.428561     1.192233     118.72
 H       4.294431    -0.609375     1.926950      24.18
 H       5.660482     0.662427     1.429562      24.82
 H       5.939130    -1.221089     1.408750      25.17
 C       3.765534    -0.116585    -1.962000      25.58
 O       4.280170    -1.140026    -2.541531     184.34
 H       5.068038    -1.585490    -1.870203      21.11
 C       2.821528     0.744314    -2.718384      68.52
 H       2.715473     0.566309    -3.886601      19.31
 C       2.593450     2.312259    -0.952543      33.12
 C       2.157645     3.689409    -0.307428      93.24
 H       2.523808     4.331692    -1.319746      17.43
 O       2.681357     4.132899     0.935620     287.15
 H       3.689650     4.295014     0.920432      27.36
 C       0.587226     3.793116    -0.385434      67.03
 H       0.161746     3.309089    -1.204264      22.01
 C      -0.112478     5.158044    -0.278826     110.07
 O       0.349223     6.281993    -1.030779     290.78
 H      -0.018087     6.215004    -1.922082      29.22
 H       0.020879     5.562361     0.682041      25.21
 H      -1.249937     5.106314    -0.111794      24.24
 C      -1.006401    -0.262247    -0.362992      48.37
 H      -0.430739    -1.225257    -0.751160      18.87
 C      -3.067686     0.927323     0.204025      62.57
 H      -4.153161     0.856770     0.342317      23.43
 C      -2.287310     2.090556     0.704612      -0.40
 O      -2.793555     3.288019     1.209495     199.14
 C      -4.136870     3.619311     1.313298     107.12
 H      -4.829671     3.571268     0.401969      25.58
 H      -4.961025     2.921080     2.065803      23.00
 H      -4.129831     4.855140     1.538183      23.46
 C      -0.845678     1.992672     0.364243       1.54
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 O       0.106413     3.000510     0.774118     178.13
 C      -0.166120     0.841073    -0.128568      22.35
 H       0.878208     1.065983    -0.094948      15.94
 C      -2.387608    -0.273345    -0.074435      35.51
 C      -3.259225    -1.465557    -0.519431      62.55
 H      -4.181139    -0.954755    -1.033226      20.84
 O      -2.478461    -2.302664    -1.452877     251.00
 H      -2.986566    -3.030428    -1.239097      21.20
 C      -3.901740    -2.400892     0.697819      94.68
 H      -3.136834    -2.829488     1.413352      19.45
 O      -4.783869    -1.509394     1.532381     286.43
 H      -4.777186    -1.965488     2.372977      28.00
 C      -4.860194    -3.428539     0.139646      81.96
 O      -4.387788    -4.166397    -0.986098     311.89
 H      -3.773706    -4.734463    -0.376102      26.88
 H      -5.610426    -2.589684    -0.287087      26.53
 H      -5.193128    -4.083636     0.924130      28.76
55
name = lig-etoh-frame_365
 C       2.201184     1.872029    -2.216194      81.39
 H       1.567901     2.449516    -2.903900      23.64
 C       3.357488     1.558853    -0.108325      73.53
 H       3.664697     2.018863     0.736716      25.79
 C       4.070843     0.389989    -0.666426      15.19
 O       4.867254    -0.575518    -0.089885     246.31
 C       5.173425    -0.455232     1.295021     121.91
 H       4.307803    -0.607977     1.871896      27.41
 H       5.526879     0.519598     1.328332      26.24
 H       5.850164    -1.279042     1.543815      25.40
 C       3.677018    -0.074711    -2.014076      20.11
 O       4.326508    -1.167699    -2.533908     224.36
 H       4.901837    -1.662501    -1.953925      25.06
 C       2.817788     0.662175    -2.753249      61.75
 H       2.809443     0.538605    -3.794938      23.72
 C       2.521102     2.316690    -0.976847      28.38
 C       2.121375     3.767077    -0.385663      92.39
 H       2.494512     4.528570    -1.240416      20.93
 O       2.632889     4.100464     0.957899     275.45
 H       3.683782     4.191787     1.106035      26.44
 C       0.572379     3.825527    -0.399036      56.63
 H       0.141806     3.284377    -1.325791      19.42
 C      -0.110691     5.178410    -0.290246      95.39
 O       0.337136     6.301909    -1.050248     172.86
 H       0.011318     6.198435    -2.166993      24.02
 H       0.396768     5.603733     0.699861      21.53
 H      -1.191458     5.308983    -0.532406      22.11
 C      -1.004433    -0.237408    -0.363121      41.57
 H      -0.496539    -1.261751    -0.512863      20.60
 C      -3.103502     0.915417     0.236350      52.96
 H      -4.210299     0.930364     0.378455      23.79
 C      -2.255946     2.037095     0.693609      -3.82
 O      -2.823490     3.272142     1.272104     205.52
 C      -4.162113     3.603288     1.300244     138.72
 H      -4.601476     3.538983     0.306924      27.70
 H      -4.602562     3.096596     2.082453      28.44
 H      -4.209157     4.535373     1.589713      29.47
 C      -0.858659     2.027280     0.389414      15.51
 O       0.128582     2.914780     0.724513     164.58
 C      -0.228436     0.916117    -0.163815      24.03
 H       0.912346     0.844514     0.239814      16.45
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 C      -2.391202    -0.300589    -0.121094      27.63
 C      -3.254878    -1.475343    -0.484130      94.65
 H      -3.933993    -1.246167    -1.317925      20.21
 O      -2.493782    -2.306403    -1.417653     219.74
 H      -2.949265    -3.263130    -1.128520      15.39
 C      -3.951050    -2.317514     0.629514     107.35
 H      -3.170473    -2.812196     1.277982      21.26
 O      -4.730464    -1.513364     1.531492     320.55
 H      -4.675037    -2.052782     2.330038      27.39
 C      -4.867403    -3.374916     0.097673     110.94
 O      -4.345341    -4.164132    -0.903200     312.70
 H      -3.715332    -4.833858    -0.657632      31.06
 H      -5.859299    -3.112031    -0.263741      26.76
 H      -5.471553    -4.065528     0.805623      26.05
55
name = lig-etoh-frame_366
 C       2.226597     1.880386    -2.195376      57.42
 H       1.379581     2.389471    -2.696810      20.03
 C       3.375908     1.504273    -0.161049      76.26
 H       3.583362     2.145868     0.822965      20.61
 C       4.047569     0.456340    -0.690713      12.70
 O       4.928057    -0.634615    -0.140539     185.73
 C       5.142109    -0.480732     1.401341      97.12
 H       4.144973    -0.536239     1.983827      24.67
 H       5.636058     0.566098     1.604464      23.90
 H       5.900246    -1.250821     1.684368      25.11
 C       3.632851    -0.026989    -1.992658      13.20
 O       4.358545    -1.212603    -2.556828     175.64
 H       4.828359    -1.707879    -1.849296      23.47
 C       2.782110     0.636043    -2.806348      53.51
 H       2.722845     0.356150    -3.903756      23.78
 C       2.476421     2.360994    -0.928901      67.54
 C       2.086635     3.814354    -0.495166      89.34
 H       2.498209     4.854313    -0.960678      22.75
 O       2.579552     4.064315     0.978851     290.44
 H       3.491448     4.051623     0.954063      31.83
 C       0.535958     3.822055    -0.430403      76.41
 H       0.361521     3.396425    -1.405211      21.99
 C      -0.085474     5.256358    -0.245263     107.91
 O       0.346470     6.342612    -1.135167     285.94
 H       0.234013     6.047122    -1.957456      35.21
 H       0.210424     5.426319     0.743763      25.61
 H      -1.169772     5.074701    -0.555190      23.45
 C      -0.999165    -0.252414    -0.349100      34.83
 H      -0.534086    -1.240813    -0.432273      21.21
 C      -3.083341     0.920186     0.305459      56.36
 H      -4.138934     0.995185     0.424075      22.36
 C      -2.280998     2.008759     0.659999       7.73
 O      -2.778556     3.226736     1.316322     171.83
 C      -4.198550     3.571409     1.265269      90.04
 H      -4.522949     3.406081     0.177231      24.46
 H      -4.689204     2.902991     2.280154      22.38
 H      -4.263022     4.744576     1.743083      22.97
 C      -0.877385     2.051714     0.414962      23.12
 O       0.149212     2.893197     0.694819     174.81
 C      -0.299709     0.931182    -0.147540      40.12
 H       0.623294     0.625110     0.076454      21.04
 C      -2.427969    -0.272543    -0.178373      17.41
 C      -3.260566    -1.483262    -0.501606      92.98
 H      -4.050558    -1.155668    -1.238066      21.84
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 O      -2.492268    -2.361091    -1.359652     272.87
 H      -2.686600    -3.297110    -1.457319      20.03
 C      -3.986020    -2.228364     0.586125      88.93
 H      -3.116453    -2.785297     1.020514      20.78
 O      -4.686824    -1.506985     1.520315     312.93
 H      -4.521017    -1.932424     2.545647      23.59
 C      -4.966620    -3.351735     0.084113      89.62
 O      -4.275954    -4.200450    -0.874651     305.94
 H      -3.722353    -4.990680    -0.680695      30.50
 H      -5.975818    -3.213800    -0.466621      25.69
 H      -5.263768    -3.934112     0.971152      27.56
55
name = lig-etoh-frame_367
 C       2.214963     1.865657    -2.238067      55.08
 H       1.372877     2.332666    -2.725146      19.37
 C       3.398404     1.546888    -0.161090      61.14
 H       3.627272     1.765934     0.842294      21.29
 C       4.026121     0.421313    -0.730750       7.45
 O       4.972640    -0.646550    -0.140048     174.86
 C       5.120778    -0.477761     1.473701     106.93
 H       4.155667    -0.499918     1.953865      26.04
 H       5.628885     0.390165     1.856886      26.75
 H       5.805414    -1.246418     1.784035      26.75
 C       3.672677    -0.055236    -1.979830      11.66
 O       4.354307    -1.224549    -2.574999     145.94
 H       4.743004    -1.696164    -1.632735      18.62
 C       2.717593     0.684620    -2.852050      44.82
 H       2.426932     0.192557    -3.829946      22.16
 C       2.499402     2.392532    -0.890048      65.80
 C       2.055857     3.843612    -0.511333      93.67
 H       2.473297     4.821261    -1.020481      22.60
 O       2.505469     4.022463     0.976880     233.60
 H       3.542449     3.985828     0.769868      26.38
 C       0.533342     3.834855    -0.467979      69.24
 H       0.243455     3.450898    -1.492398      20.16
 C      -0.078657     5.301526    -0.222143      93.43
 O       0.377602     6.385147    -1.185361     215.41
 H       0.345914     5.746079    -2.216260      21.35
 H      -0.150953     5.537176     0.951550      22.72
 H      -1.141779     4.952699    -0.182463      23.56
 C      -1.069538    -0.285095    -0.328357      40.55
 H      -0.412172    -1.308416    -0.526955      16.98
 C      -3.037558     0.907419     0.366417      65.51
 H      -4.153905     0.978381     0.512063      19.34
 C      -2.313741     2.062325     0.649346      19.66
 O      -2.720584     3.169032     1.340182     203.03
 C      -4.218854     3.532842     1.293657     131.25
 H      -4.646832     3.357883     0.342615      29.09
 H      -4.849837     2.885597     1.803864      28.57
 H      -4.274911     4.493561     1.499397      28.90
 C      -0.899072     2.036573     0.413333      20.82
 O       0.171715     2.950055     0.673449     168.55
 C      -0.385583     0.862154    -0.109971      26.24
 H       0.844109     0.679478    -0.222333      16.77
 C      -2.460935    -0.223013    -0.227475      25.62
 C      -3.312862    -1.472590    -0.596675      84.49
 H      -4.209613    -0.899945    -1.008388      21.65
 O      -2.442557    -2.412088    -1.315667     242.35
 H      -2.817009    -3.278356    -1.503819      19.74
 C      -4.007286    -2.207715     0.552721      75.87
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 H      -3.128402    -2.861711     0.879241      18.65
 O      -4.660520    -1.473579     1.551774     405.02
 H      -4.257381    -1.551040     2.377487      31.82
 C      -5.062309    -3.370449     0.077307      69.04
 O      -4.204674    -4.261719    -0.889737     246.22
 H      -3.900269    -5.022543    -0.240721      27.33
 H      -5.828101    -2.943419    -0.543308      27.64
 H      -5.000525    -3.790886     1.129281      27.07
55
name = lig-etoh-frame_368
 C       2.178015     1.862451    -2.279532      59.28
 H       1.432289     2.387487    -2.930020      22.37
 C       3.430327     1.604551    -0.142386      82.67
 H       3.727125     1.536496     0.975990      18.62
 C       4.022743     0.321697    -0.753182      25.84
 O       4.996906    -0.599165    -0.075325     202.32
 C       5.108048    -0.481316     1.495997     102.33
 H       4.062759    -0.565639     1.902595      25.43
 H       5.633255     0.467786     1.845808      26.75
 H       5.617817    -1.455683     1.810524      25.47
 C       3.707510    -0.102213    -2.069915      19.47
 O       4.318898    -1.213235    -2.544245     248.88
 H       4.684601    -1.635272    -1.848858      27.17
 C       2.688342     0.711664    -2.826328      53.37
 H       2.160040     0.259241    -3.646500      21.77
 C       2.571158     2.394230    -0.923617      44.68
 C       2.031920     3.829544    -0.436154     106.31
 H       2.476189     4.528133    -1.344582      18.72
 O       2.449841     3.985422     0.931876     272.92
 H       3.477106     4.027178     0.891154      27.09
 C       0.542616     3.891072    -0.493611      72.83
 H      -0.060947     3.524412    -1.350657      19.36
 C      -0.098690     5.313204    -0.180092      88.74
 O       0.398763     6.370081    -1.233696     252.84
 H       0.276455     5.940097    -2.040404      30.88
 H      -0.030228     5.840732     0.758608      24.21
 H      -1.241823     5.133000    -0.168462      23.62
 C      -1.142603    -0.366393    -0.323219      55.81
 H      -0.625325    -1.143949    -0.655061      19.42
 C      -3.033705     0.905618     0.409336      67.99
 H      -4.072776     0.863486     0.606818      18.28
 C      -2.290454     2.127430     0.653775      18.49
 O      -2.718989     3.139796     1.363812     186.59
 C      -4.197685     3.451797     1.283696      95.24
 H      -4.658492     3.382528     0.203143      25.20
 H      -5.050550     2.687871     1.867279      22.72
 H      -4.286669     4.668271     1.485599      23.54
 C      -0.893124     2.006623     0.389990       4.30
 O       0.162276     3.033807     0.645115     181.48
 C      -0.372905     0.772591    -0.065336      37.11
 H       0.527170     1.011532    -0.421474      17.94
 C      -2.502347    -0.224102    -0.258852      22.22
 C      -3.385311    -1.415522    -0.690161      76.00
 H      -4.230018    -0.949273    -1.245343      21.52
 O      -2.390875    -2.439266    -1.289024     165.35
 H      -3.234510    -3.158450    -1.332144      13.79
 C      -4.004468    -2.255282     0.520892      84.02
 H      -3.245395    -2.859224     0.997976      19.53
 O      -4.646581    -1.417081     1.576241     349.12
 H      -3.855141    -1.278365     2.359081      22.47
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 C      -5.050488    -3.363763     0.062656      66.53
 O      -4.162887    -4.347703    -0.871059     261.05
 H      -4.070602    -4.804600    -0.051526      25.98
 H      -5.880986    -2.789544    -0.434099      26.73
 H      -5.285027    -3.859625     1.040179      27.56
55
name = lig-etoh-frame_369
 C       2.152244     1.901492    -2.279326      33.33
 H       1.562345     2.480369    -2.973130      22.27
 C       3.498719     1.569021    -0.151273      74.14
 H       3.671401     1.731534     0.955175      18.21
 C       4.014528     0.257046    -0.741699      29.68
 O       5.000176    -0.518840     0.013736     223.54
 C       5.077000    -0.503690     1.477062     116.63
 H       4.025831    -0.521584     1.842760      27.67
 H       5.615415     0.430053     1.716185      27.92
 H       5.475887    -1.448464     1.734733      26.98
 C       3.704786    -0.094081    -2.142817      18.27
 O       4.266157    -1.215192    -2.549341     204.17
 H       4.843379    -1.748022    -1.831508      20.13
 C       2.699892     0.680653    -2.764218      64.48
 H       1.992227     0.328839    -3.630937      20.06
 C       2.633388     2.388471    -0.993511      45.27
 C       2.045575     3.744855    -0.409738     115.72
 H       2.498012     4.418288    -1.282175      18.30
 O       2.416749     3.975383     0.882141     312.12
 H       3.316037     4.068569     1.037282      31.54
 C       0.499244     3.973253    -0.465336      71.69
 H      -0.036373     3.604543    -1.326990      19.92
 C      -0.122810     5.357375    -0.182517      94.07
 O       0.406201     6.346852    -1.215259     152.00
 H       0.112321     5.928999    -2.328998      20.83
 H       0.403712     5.976993     0.676046      21.03
 H      -1.186655     5.372184    -0.388381      23.26
 C      -1.178337    -0.412796    -0.321646      21.45
 H      -0.755349    -1.403263    -1.020683      14.32
 C      -3.043169     0.931346     0.425562      57.85
 H      -4.115737     0.830054     0.753456      17.14
 C      -2.231560     2.099401     0.651064       8.64
 O      -2.780619     3.163285     1.401352     201.92
 C      -4.203715     3.384186     1.243056     129.08
 H      -4.361470     3.364111     0.215501      27.82
 H      -4.701412     2.833909     1.994225      26.65
 H      -4.272647     4.346745     1.654687      27.45
 C      -0.854014     1.990443     0.368746       8.72
 O       0.098642     3.090714     0.624039     176.61
 C      -0.362220     0.730561    -0.019745      27.89
 H       0.653519     1.011391    -0.619209      15.50
 C      -2.577746    -0.250250    -0.256369      23.14
 C      -3.424488    -1.363465    -0.742481      69.61
 H      -4.103392    -1.266814    -1.684762      19.75
 O      -2.411161    -2.450629    -1.275861     174.18
 H      -2.989173    -3.171287    -1.261317      19.97
 C      -4.015858    -2.291653     0.511028      80.61
 H      -3.160528    -2.774882     1.139236      19.03
 O      -4.619119    -1.366600     1.593845     322.78
 H      -3.756953    -1.180940     2.124201      23.97
 C      -5.003240    -3.316611     0.040803      92.16
 O      -4.179495    -4.414644    -0.817793     233.88
 H      -3.817341    -4.922587     0.015447      24.86
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 H      -5.935875    -2.954548    -0.403221      26.52
 H      -5.652014    -3.979375     0.761531      26.01
55
name = lig-etoh-frame_370
 C       2.189302     1.937323    -2.240044      34.14
 H       1.591411     2.587605    -2.911708      19.52
 C       3.554616     1.482674    -0.221999      35.41
 H       3.649708     1.972705     0.777905      17.66
 C       4.004757     0.279400    -0.689139      30.72
 O       4.983340    -0.443947     0.055137     254.25
 C       5.009273    -0.507271     1.430256     117.20
 H       4.015503    -0.380491     1.900276      27.67
 H       5.651884     0.327338     1.804883      26.87
 H       5.572283    -1.470378     1.734485      25.77
 C       3.692898    -0.051954    -2.095697      15.67
 O       4.219499    -1.272048    -2.595694     171.60
 H       4.942691    -1.611304    -1.872629      21.08
 C       2.671457     0.644205    -2.736110      66.45
 H       2.273569     0.287468    -3.617836      25.22
 C       2.669062     2.364567    -1.039382      56.62
 C       2.075843     3.648348    -0.477475     104.02
 H       2.562675     4.637937    -0.975142      20.15
 O       2.387167     3.983523     0.878003     248.47
 H       3.440336     4.129555     1.074349      26.52
 C       0.436775     4.018322    -0.419781      60.80
 H       0.197955     3.663982    -1.486924      18.65
 C      -0.076614     5.461199    -0.225258     108.87
 O       0.403149     6.312236    -1.229869     294.63
 H       0.123206     5.986239    -2.061668      31.59
 H       0.478731     5.702744     0.694941      23.93
 H      -1.240330     5.527947    -0.252267      23.40
 C      -1.184788    -0.444698    -0.363580      25.15
 H      -0.934325    -1.180598    -0.900044      18.19
 C      -3.071296     0.949323     0.417477      52.98
 H      -4.055121     0.998269     0.854609      18.88
 C      -2.207607     2.035061     0.683062      -4.06
 O      -2.815878     3.183550     1.419979     174.16
 C      -4.169505     3.337424     1.225170      95.38
 H      -4.404034     3.246622     0.057115      24.22
 H      -4.716220     2.586239     2.078431      22.79
 H      -4.369675     4.403990     1.755890      23.81
 C      -0.797034     1.998517     0.367199      18.45
 O      -0.014235     3.108829     0.623074     215.92
 C      -0.321143     0.713489    -0.031874      37.89
 H       0.632976     0.496321    -0.437802      19.28
 C      -2.627165    -0.249499    -0.227243      17.97
 C      -3.441026    -1.412015    -0.782443      69.32
 H      -3.949603    -1.405830    -1.703988      20.10
 O      -2.441798    -2.437676    -1.275410     134.49
 H      -2.798959    -3.481406    -1.274630      15.94
 C      -4.034365    -2.258171     0.545580      77.86
 H      -3.139575    -2.660864     0.912486      24.15
 O      -4.590113    -1.335485     1.568834     373.40
 H      -3.878266    -1.180687     2.143240      30.87
 C      -4.984057    -3.329877     0.018651      82.27
 O      -4.225676    -4.463360    -0.727165     272.30
 H      -3.532915    -4.962050    -0.210289      28.49
 H      -5.738530    -2.998436    -0.796881      24.53
 H      -5.625005    -3.960788     0.645943      24.12
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```
name = lig-etoh-frame_371
 C       2.251047     1.926167    -2.250354      45.41
 H       1.568597     2.580649    -2.785908      19.00
 C       3.541750     1.479586    -0.296917      38.11
 H       3.869039     2.060598     0.669509      17.99
 C       4.025079     0.312338    -0.645051      33.94
 O       4.955856    -0.391138     0.023290     274.47
 C       4.962078    -0.492764     1.434066     121.35
 H       3.990801    -0.340136     1.988046      26.35
 H       5.660509     0.223376     1.970738      26.09
 H       5.457593    -1.399642     1.690710      27.41
 C       3.683006    -0.058816    -1.989570       9.40
 O       4.176008    -1.315698    -2.634720     205.57
 H       4.842992    -1.505749    -2.083772      27.23
 C       2.639930     0.641313    -2.714954      55.60
 H       2.579545     0.173206    -3.818628      24.84
 C       2.696148     2.326408    -1.030227      42.24
 C       2.105052     3.654911    -0.524316      90.99
 H       2.556320     4.635975    -1.029101      22.12
 O       2.391644     3.985021     0.923502     277.64
 H       3.356549     4.134022     0.904013      28.16
 C       0.411516     3.980146    -0.440716      53.79
 H       0.171217     3.676462    -1.419198      19.86
 C      -0.018393     5.528602    -0.244364     106.43
 O       0.423265     6.319475    -1.231991     276.59
 H       0.079288     5.815603    -2.276325      20.20
 H       0.337787     5.705604     0.855561      22.61
 H      -1.079742     5.525615     0.091352      23.56
 C      -1.235692    -0.356611    -0.365957      30.37
 H      -0.751496    -1.393566    -0.941971      16.54
 C      -3.098308     0.953174     0.403478      72.59
 H      -4.091984     1.125542     0.805376      21.39
 C      -2.207985     1.986277     0.743430      -3.51
 O      -2.778360     3.174113     1.401333     220.80
 C      -4.178259     3.301488     1.252628     135.77
 H      -4.617827     3.178627     0.314422      29.21
 H      -4.781482     2.487618     1.594143      28.32
 H      -4.555318     4.293846     1.519914      27.27
 C      -0.772919     1.982041     0.374029      15.60
 O      -0.136062     3.131012     0.633870     204.95
 C      -0.297109     0.659180    -0.075883      38.00
 H       0.788706     0.225366    -0.148057      18.98
 C      -2.620341    -0.245869    -0.212256      26.10
 C      -3.431918    -1.533141    -0.768259      60.17
 H      -4.202929    -1.180045    -1.622253      21.28
 O      -2.455247    -2.437755    -1.294073     174.88
 H      -2.794388    -3.422328    -1.211169      18.23
 C      -4.063852    -2.167608     0.560315      61.02
 H      -3.029693    -2.706206     0.777635      20.35
 O      -4.576608    -1.325223     1.507380     332.41
 H      -3.958990    -1.297071     2.482832      21.93
 C      -4.983362    -3.393825    -0.034557      68.52
 O      -4.266524    -4.501423    -0.650018     301.00
 H      -3.513984    -4.827301    -0.153115      30.60
 H      -5.275588    -2.988719    -1.007272      25.38
 H      -5.564688    -3.801850     0.871555      24.19
55
name = lig-etoh-frame_372
 C       2.291306     1.880693    -2.313719      50.97
 H       1.528175     2.490994    -2.804750      18.35
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 C       3.516818     1.603283    -0.277961      42.61
 H       4.058671     1.889773     0.585605      20.31
 C       4.049298     0.307021    -0.676265      24.46
 O       4.953908    -0.371984    -0.010967     256.80
 C       4.936353    -0.458292     1.489122     104.55
 H       3.934581    -0.403837     1.897677      26.15
 H       5.604532     0.265077     1.926718      25.79
 H       5.244440    -1.558991     1.643487      24.73
 C       3.636871    -0.125280    -1.922890      18.85
 O       4.107101    -1.309880    -2.653902     147.24
 H       5.046687    -1.673149    -2.155459      21.88
 C       2.673941     0.618425    -2.720225      62.53
 H       2.663586     0.323560    -3.697201      28.53
 C       2.684404     2.325124    -1.000642      51.10
 C       2.101029     3.727211    -0.493236      84.78
 H       2.504230     4.463558    -1.364701      23.73
 O       2.417665     3.974423     0.952983     277.22
 H       3.357547     4.153234     0.923984      28.74
 C       0.436900     3.912866    -0.481178      52.45
 H      -0.183414     3.548063    -1.414259      19.74
 C       0.037285     5.494459    -0.172024      86.93
 O       0.444113     6.351780    -1.289772     267.15
 H       0.260825     5.817251    -2.078716      30.41
 H       0.481161     5.997509     0.760575      23.32
 H      -1.092770     5.460243     0.100486      23.68
 C      -1.252950    -0.290660    -0.389442      59.53
 H      -0.790875    -1.163287    -0.578782      21.11
 C      -3.115997     0.939926     0.393215      73.31
 H      -4.215102     1.022062     0.566407      21.53
 C      -2.205662     1.957142     0.792644       2.49
 O      -2.715447     3.144344     1.352834     175.67
 C      -4.225913     3.261868     1.255723      91.51
 H      -4.605119     3.224087     0.111014      25.28
 H      -4.893292     2.340059     1.694507      23.30
 H      -4.580887     4.273726     1.566058      26.21
 C      -0.812395     1.901577     0.385189       5.00
 O      -0.228486     3.183489     0.645422     169.09
 C      -0.270602     0.628467    -0.107798      53.87
 H       0.777492     0.396531     0.178220      17.91
 C      -2.611426    -0.257141    -0.225508      19.74
 C      -3.432038    -1.574687    -0.721085      85.27
 H      -4.230117    -1.100352    -1.215651      22.87
 O      -2.468569    -2.449035    -1.330825     260.79
 H      -2.931461    -3.269117    -1.214845      19.79
 C      -4.026082    -2.154502     0.512543      89.08
 H      -3.233888    -2.666932     0.992071      22.08
 O      -4.568767    -1.306487     1.485069     385.76
 H      -4.267363    -1.608133     2.290137      30.29
 C      -4.966073    -3.438779    -0.061806      74.21
 O      -4.281904    -4.552407    -0.581343     318.13
 H      -3.626257    -4.737530     0.214683      27.66
 H      -5.401604    -2.938168    -0.955724      28.03
 H      -5.691099    -3.457708     0.802880      26.38
55
name = lig-etoh-frame_373
 C       2.302909     1.847700    -2.345331      30.45
 H       1.562279     2.350231    -3.001738      17.29
 C       3.561081     1.665260    -0.210825      90.61
 H       4.188061     1.933947     0.785544      19.62
 C       4.017088     0.354029    -0.737880      22.44
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 O       4.994333    -0.386644    -0.004459     221.95
 C       4.909624    -0.455169     1.519357      94.94
 H       3.803339    -0.324398     1.765764      22.85
 H       5.612542     0.359209     1.907925      22.84
 H       5.114752    -1.500352     1.678752      24.48
 C       3.571966    -0.232117    -1.929357      32.03
 O       4.054679    -1.288781    -2.635746     223.75
 H       4.865042    -1.800053    -2.383119      24.73
 C       2.762790     0.594297    -2.714730      57.17
 H       2.519944     0.333397    -3.840689      23.90
 C       2.598879     2.396755    -1.002775      60.09
 C       2.051722     3.760371    -0.454587     103.54
 H       2.436525     4.463104    -1.225166      23.55
 O       2.453495     3.970305     0.938831     248.13
 H       3.506802     4.185181     1.093505      25.92
 C       0.464108     3.859779    -0.496531      64.59
 H      -0.159838     3.565704    -1.273723      21.24
 C       0.095117     5.434179    -0.108576      83.01
 O       0.468051     6.391668    -1.308897     137.08
 H       0.247732     5.770656    -2.318965      21.53
 H       0.736762     6.016247     0.617773      22.15
 H      -0.990127     5.426629    -0.132727      23.65
 C      -1.222641    -0.271181    -0.401205      40.69
 H      -0.761379    -1.420775    -0.469950      17.45
 C      -3.135269     0.891817     0.370179      85.47
 H      -4.193963     0.902239     0.351494      21.40
 C      -2.224449     1.918781     0.802050       5.76
 O      -2.687494     3.114255     1.295929     149.31
 C      -4.291799     3.204954     1.206842      92.74
 H      -4.321458     3.293012     0.191709      26.50
 H      -4.676215     2.522267     1.986763      24.51
 H      -4.362986     4.201039     1.840791      25.50
 C      -0.874784     1.838328     0.415174       8.22
 O      -0.290173     3.222624     0.653097     131.74
 C      -0.261178     0.698367    -0.078783      56.98
 H       0.779185     0.562343     0.154481      17.92
 C      -2.621672    -0.256029    -0.248408      24.27
 C      -3.384126    -1.489079    -0.628163      72.33
 H      -4.343189    -1.156265    -1.272624      19.87
 O      -2.501143    -2.458505    -1.379321     173.07
 H      -3.113918    -3.419099    -1.349333      13.99
 C      -3.966983    -2.253331     0.473868      89.14
 H      -3.257340    -2.745795     1.255149      17.04
 O      -4.596626    -1.280777     1.446709     295.88
 H      -4.421127    -1.842539     2.319719      23.41
 C      -4.981044    -3.373910    -0.077652      86.22
 O      -4.265394    -4.615746    -0.480044     284.77
 H      -3.889915    -4.891034     0.388657      28.42
 H      -5.756585    -3.020362    -0.813151      27.62
 H      -5.847390    -3.515374     0.634845      27.92
55
name = lig-etoh-frame_374
 C       2.294927     1.843984    -2.317589      46.16
 H       1.714666     2.253883    -3.140462      23.38
 C       3.616658     1.675833    -0.174939      43.17
 H       3.950288     2.089617     0.686971      20.40
 C       3.993737     0.416832    -0.736762      -5.09
 O       5.034352    -0.405131     0.009524     214.59
 C       4.859081    -0.435563     1.494477     103.50
 H       3.868938    -0.124048     1.745005      25.80
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 H       5.515263     0.250092     1.979976      26.15
 H       5.197437    -1.456825     1.879636      25.29
 C       3.521428    -0.295230    -1.948913      33.08
 O       4.004960    -1.308267    -2.635134     243.06
 H       4.706965    -1.818131    -2.281730      27.27
 C       2.828996     0.588914    -2.762484      53.72
 H       2.400147     0.231158    -3.681717      21.32
 C       2.537499     2.453142    -1.005374      41.52
 C       1.993170     3.726573    -0.424601     101.98
 H       2.403455     4.826436    -0.932258      18.59
 O       2.498214     3.978616     0.918601     288.45
 H       3.422024     4.111032     1.004328      31.27
 C       0.484781     3.867300    -0.420327      71.80
 H       0.111400     3.570291    -1.502450      19.34
 C       0.172100     5.377257    -0.152384      80.82
 O       0.490584     6.395611    -1.326326     192.84
 H       0.152318     6.052392    -2.171889      28.29
 H       0.862737     5.742202     0.746786      22.97
 H      -0.972721     5.494162    -0.078449      22.82
 C      -1.139021    -0.344736    -0.393239      41.16
 H      -0.836470    -1.382147    -0.541163      20.27
 C      -3.149969     0.837750     0.336440      66.87
 H      -4.272743     0.955035     0.348117      19.95
 C      -2.293141     1.865888     0.771489       7.92
 O      -2.702104     3.085244     1.244089     156.27
 C      -4.256736     3.198616     1.236397     100.02
 H      -4.471477     3.273299     0.053130      24.41
 H      -4.656096     2.416109     1.955402      25.68
 H      -4.283656     4.099259     1.746604      27.32
 C      -0.919478     1.878763     0.471645      14.37
 O      -0.326846     3.217166     0.656719     150.19
 C      -0.281684     0.779389    -0.024000      47.48
 H       0.895087     0.659706    -0.176854      17.76
 C      -2.573530    -0.239472    -0.272256      33.33
 C      -3.343789    -1.398968    -0.592068      88.46
 H      -4.104767    -1.283167    -1.279971      22.84
 O      -2.567144    -2.478017    -1.432156     257.12
 H      -2.980853    -3.264786    -1.468764      23.37
 C      -3.948715    -2.377481     0.516267      73.38
 H      -3.182331    -2.892072     1.061416      19.74
 O      -4.636586    -1.283275     1.393734     271.45
 H      -4.650703    -1.725286     2.396174      24.80
 C      -5.033782    -3.287876    -0.066655      92.24
 O      -4.268030    -4.660946    -0.375632     238.87
 H      -3.973024    -5.105318     0.464886      28.31
 H      -5.692340    -3.110160    -0.948293      28.08
 H      -5.695117    -3.808859     0.715734      26.69
55
name = lig-etoh-frame_375
 C       2.289358     1.852319    -2.268716      64.60
 H       1.778362     2.397196    -3.097832      23.92
 C       3.587858     1.680563    -0.246539      35.26
 H       3.838003     2.247615     0.789261      15.99
 C       4.021037     0.423690    -0.678975       1.27
 O       5.045952    -0.410712     0.020568     252.04
 C       4.826607    -0.416748     1.447317     103.65
 H       3.815040    -0.026303     1.796633      24.44
 H       5.539410     0.305124     2.023036      24.59
 H       5.109687    -1.339168     1.998501      25.93
 C       3.496646    -0.241066    -1.932573      18.15
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 O       3.972947    -1.385955    -2.651598     161.38
 H       4.628174    -1.899642    -1.868195      21.71
 C       2.829903     0.619558    -2.795508      48.38
 H       2.391782     0.118672    -3.704742      19.59
 C       2.557361     2.433271    -1.016333      37.21
 C       1.982055     3.722502    -0.383989     107.45
 H       2.226547     4.727560    -0.904280      20.57
 O       2.523896     3.977422     0.919484     264.05
 H       3.519789     4.059672     0.778619      29.95
 C       0.471201     3.891715    -0.363051      84.89
 H       0.443086     3.581096    -1.376400      21.28
 C       0.227529     5.357848    -0.241870     111.32
 O       0.526511     6.398112    -1.276327     244.58
 H       0.053963     5.977921    -2.239769      21.95
 H       0.745326     5.520814     0.722360      25.25
 H      -0.766381     5.516502     0.172756      24.78
 C      -1.062301    -0.388276    -0.347016      43.82
 H      -0.650196    -1.430993    -0.722835      16.96
 C      -3.181737     0.823032     0.305906      62.46
 H      -4.213952     0.949043     0.439193      19.02
 C      -2.369530     1.838566     0.721937      11.70
 O      -2.772880     3.056951     1.198496     226.35
 C      -4.153421     3.199726     1.259498     129.58
 H      -4.813355     3.157116     0.403453      27.68
 H      -4.755042     2.267541     1.629041      25.56
 H      -4.441341     4.323392     1.643643      24.28
 C      -0.933096     1.977736     0.525886       8.64
 O      -0.345071     3.186198     0.656423     187.02
 C      -0.288195     0.791048     0.000874      42.14
 H       0.637804     0.853317    -0.408601      19.66
 C      -2.442251    -0.246894    -0.289792      41.19
 C      -3.326308    -1.453224    -0.601393      66.68
 H      -4.186918    -1.087122    -1.363755      20.73
 O      -2.603479    -2.455408    -1.491524     205.52
 H      -3.124416    -3.400331    -1.414647      16.37
 C      -3.976814    -2.392578     0.567221      59.50
 H      -3.110205    -3.049998     0.918559      17.39
 O      -4.681604    -1.327281     1.347881     355.49
 H      -4.738210    -1.429999     2.218418      31.36
 C      -5.064810    -3.313002    -0.012340      85.19
 O      -4.301877    -4.682066    -0.316615     209.32
 H      -3.909638    -5.075544     0.573919      25.28
 H      -5.376902    -3.043467    -1.042751      27.47
 H      -5.592493    -3.659557     0.826458      27.63
55
name = lig-etoh-frame_376
 C       2.276861     1.877799    -2.274227      83.64
 H       1.705947     2.596761    -2.854171      23.38
 C       3.521254     1.704615    -0.310976      92.03
 H       3.846728     2.002496     0.598903      21.54
 C       4.070883     0.366803    -0.638861      15.90
 O       5.020461    -0.400829     0.024920     271.40
 C       4.818668    -0.359042     1.453393     111.94
 H       3.809047    -0.092100     1.697618      25.48
 H       5.499358     0.366521     1.799925      25.93
 H       4.924369    -1.391918     1.862097      25.06
 C       3.527732    -0.144359    -1.918989      27.98
 O       3.961228    -1.472966    -2.599528     207.65
 H       4.346454    -1.908761    -1.890573      28.98
 C       2.771951     0.666692    -2.790451      32.73
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 H       2.500490     0.203830    -3.800844      16.87
 C       2.627784     2.372608    -1.015772       3.35
 C       2.003321     3.715454    -0.323439      90.33
 H       2.156277     4.481320    -1.291824      19.72
 O       2.566216     3.973064     0.936229     241.57
 H       3.604947     4.061085     0.671582      27.90
 C       0.471621     3.876891    -0.356692      73.08
 H       0.189625     3.418209    -1.385481      19.87
 C       0.234680     5.394236    -0.283274     101.78
 O       0.554354     6.370265    -1.218118     265.82
 H       0.256566     5.881979    -2.101023      26.98
 H       0.918378     5.650133     0.698191      23.50
 H      -0.795629     5.514988     0.257670      23.67
 C      -0.984216    -0.399324    -0.275204      52.25
 H      -0.388745    -1.174989    -0.926768      17.30
 C      -3.166491     0.807347     0.262830      73.37
 H      -4.278363     0.735117     0.425748      18.64
 C      -2.385293     1.875646     0.675325      11.44
 O      -2.864921     3.044036     1.155834     233.73
 C      -4.148590     3.227084     1.286648     141.26
 H      -4.824004     3.175052     0.315196      26.38
 H      -4.638224     2.369234     1.818841      26.71
 H      -4.433991     4.087285     1.685803      28.58
 C      -0.942863     1.977101     0.524950      11.88
 O      -0.340988     3.185696     0.664042     174.38
 C      -0.318257     0.804284     0.020876      31.64
 H       0.689689     1.074117    -0.587228      15.02
 C      -2.360723    -0.325883    -0.279531      29.80
 C      -3.335480    -1.559920    -0.670159      79.48
 H      -4.119654    -0.960120    -1.062574      23.66
 O      -2.642207    -2.439531    -1.553236     256.22
 H      -3.125234    -3.327383    -1.232902      16.14
 C      -4.008774    -2.320923     0.587425      89.24
 H      -3.206733    -2.935491     1.058680      19.97
 O      -4.726268    -1.386584     1.281176     316.06
 H      -4.645486    -1.293694     2.378429      24.80
 C      -5.018315    -3.416143     0.053460      62.77
 O      -4.366149    -4.680941    -0.284622     310.36
 H      -3.779778    -4.828568     0.488666      28.79
 H      -5.314559    -2.951347    -0.910181      27.37
 H      -5.961409    -3.295246     0.852478      25.13
55
name = lig-etoh-frame_377
 C       2.248767     1.934347    -2.317558      26.39
 H       1.536590     2.643712    -2.780202      13.40
 C       3.546044     1.614821    -0.311423      27.39
 H       3.946564     1.956398     0.726068      16.06
 C       4.071928     0.323328    -0.687257      39.76
 O       4.975484    -0.388419     0.019330     263.23
 C       4.813271    -0.309143     1.472302      98.32
 H       3.730520    -0.026520     1.617685      23.30
 H       5.578451     0.465040     1.826819      24.93
 H       4.918078    -1.407976     1.715243      24.37
 C       3.612270    -0.094669    -1.927037      33.70
 O       3.927225    -1.500659    -2.514522     181.01
 H       4.317921    -2.110585    -1.792567      23.14
 C       2.704232     0.707369    -2.769126      63.51
 H       2.573925     0.434047    -3.778400      31.06
 C       2.643680     2.362172    -1.014243      65.79
 C       2.027943     3.655987    -0.340596     111.27
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 H       2.297283     4.357622    -1.233057      24.12
 O       2.635086     3.981578     0.935238     304.75
 H       3.542599     4.073843     0.910580      33.93
 C       0.474651     3.818654    -0.408939      72.01
 H      -0.118913     3.401611    -1.204062      21.19
 C       0.214712     5.443106    -0.183962     101.75
 O       0.587692     6.331212    -1.188971     219.53
 H       0.377123     5.927762    -2.161876      26.49
 H       0.975792     5.815175     0.533719      25.06
 H      -0.842117     5.537358     0.021121      25.65
 C      -0.905712    -0.383148    -0.229129      53.19
 H      -0.306996    -1.004085    -0.821181      18.97
 C      -3.094748     0.752733     0.206423      55.76
 H      -4.148522     0.524025     0.303175      16.98
 C      -2.371297     1.931040     0.630263       8.03
 O      -2.894126     3.062212     1.115404     195.29
 C      -4.300469     3.212709     1.289474     103.39
 H      -4.559653     3.252982     0.246214      24.40
 H      -4.525337     2.547247     2.247463      22.82
 H      -4.384807     4.263940     1.984341      23.33
 C      -0.967519     1.910419     0.483891      17.95
 O      -0.320516     3.218600     0.693941     158.17
 C      -0.299496     0.864834     0.012122      47.99
 H       0.615499     1.024227    -0.374015      16.20
 C      -2.372433    -0.448377    -0.232232      20.29
 C      -3.312972    -1.606399    -0.698555      67.94
 H      -4.260107    -0.989090    -1.044038      21.00
 O      -2.698763    -2.450394    -1.606278     307.24
 H      -2.936323    -3.302189    -1.378676      22.05
 C      -4.006170    -2.283554     0.571229      99.60
 H      -3.260996    -2.640551     1.382882      19.70
 O      -4.800571    -1.411546     1.259696     333.71
 H      -4.278451    -1.365492     2.156748      25.10
 C      -4.990704    -3.469216     0.119380      92.19
 O      -4.446583    -4.664334    -0.252738     332.73
 H      -3.605079    -4.781765     0.361551      27.09
 H      -5.482371    -3.034567    -0.791170      26.22
 H      -5.921762    -3.321749     0.548230      25.74
55
name = lig-etoh-frame_378
 C       2.213164     2.013611    -2.331602      22.73
 H       1.437755     2.492686    -2.944250      18.20
 C       3.621756     1.496089    -0.246661      20.46
 H       3.909020     1.975249     0.677377      18.46
 C       4.042824     0.329334    -0.767527      24.83
 O       4.940053    -0.390826     0.012722     247.41
 C       4.803303    -0.266734     1.470253     108.82
 H       3.812046     0.099843     1.729509      25.08
 H       5.511272     0.354018     1.998769      27.01
 H       5.061892    -1.248368     1.839816      26.88
 C       3.676063    -0.124620    -2.006724      17.02
 O       3.882653    -1.468169    -2.412769     193.18
 H       4.386272    -2.176149    -1.725950      20.47
 C       2.678840     0.725815    -2.732160      80.71
 H       2.540135     0.516795    -3.899116      27.39
 C       2.627192     2.364141    -1.001961      56.57
 C       2.073840     3.565211    -0.416073     106.24
 H       2.542581     4.558176    -0.961968      22.54
 O       2.668430     3.992150     0.930305     236.87
 H       3.717860     4.063436     1.014068      28.25
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 C       0.463733     3.794169    -0.409184      54.38
 H      -0.045853     3.489614    -1.360700      21.55
 C       0.190655     5.442941    -0.080029      79.20
 O       0.634842     6.307397    -1.203389     162.50
 H       0.331355     5.974822    -2.252180      24.19
 H       0.876749     5.858372     0.846636      23.55
 H      -0.941286     5.564050    -0.058888      24.41
 C      -0.896694    -0.361087    -0.207170      35.23
 H      -0.130427    -1.234210    -0.708478      17.91
 C      -2.986340     0.676580     0.157371      54.62
 H      -4.081398     0.604935     0.213257      21.45
 C      -2.379180     1.927947     0.575279       8.49
 O      -2.894986     3.109855     1.087103     164.23
 C      -4.434749     3.232471     1.366999     117.52
 H      -4.875729     3.239493     0.322592      25.63
 H      -4.763603     2.559362     2.105263      27.31
 H      -4.371677     4.177233     1.685785      27.50
 C      -0.992785     1.951452     0.456578      12.04
 O      -0.298466     3.233729     0.743064     147.90
 C      -0.258150     0.872907    -0.010406      36.30
 H       0.920265     0.942118    -0.156218      14.93
 C      -2.364975    -0.535281    -0.174163      33.59
 C      -3.314029    -1.586411    -0.665419      81.23
 H      -4.157273    -1.271182    -1.246227      21.48
 O      -2.748182    -2.471776    -1.675778     253.33
 H      -2.805799    -3.568859    -1.548963      19.32
 C      -3.973965    -2.331445     0.543127      95.22
 H      -3.264178    -2.475259     1.361297      20.77
 O      -4.881676    -1.392556     1.274301     339.70
 H      -4.312490    -1.260405     1.981097      27.51
 C      -4.984930    -3.415423     0.128801      75.16
 O      -4.490931    -4.684580    -0.221540     297.71
 H      -3.690746    -4.947930     0.256177      29.85
 H      -5.461035    -3.130195    -0.848085      24.41
 H      -5.960865    -3.716996     0.898392      22.32
55
name = lig-etoh-frame_379
 C       2.206233     2.032806    -2.307492      32.13
 H       1.486503     2.416239    -3.034950      18.31
 C       3.601793     1.500968    -0.222996      29.65
 H       3.973490     1.884566     0.718171      18.43
 C       4.053659     0.330947    -0.804608      13.07
 O       4.918860    -0.416732     0.015081     231.90
 C       4.800905    -0.236883     1.465538      99.77
 H       3.829063     0.108220     1.880388      24.39
 H       5.549430     0.466432     1.966813      25.38
 H       5.087778    -1.206484     2.035800      25.56
 C       3.665983    -0.162637    -2.124232      22.78
 O       3.844500    -1.434072    -2.325853     247.86
 H       4.409872    -1.780644    -1.738407      25.23
 C       2.702203     0.722484    -2.745975      84.62
 H       2.423513     0.439153    -3.681817      28.37
 C       2.645331     2.308623    -0.986171      53.59
 C       2.140487     3.572987    -0.450012      98.41
 H       2.494080     4.517262    -0.976144      23.43
 O       2.683337     3.987580     0.937942     245.35
 H       3.705008     3.958697     0.809305      28.71
 C       0.463011     3.833364    -0.354378      57.98
 H       0.242554     3.632704    -1.417065      20.80
 C       0.172805     5.415057    -0.037101      93.81
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 O       0.687238     6.290577    -1.221437     239.62
 H       0.254994     5.863720    -1.968065      31.24
 H       0.529180     5.683728     0.950609      26.09
 H      -0.884972     5.535247     0.116136      26.08
 C      -0.890348    -0.403045    -0.226372      51.90
 H      -0.344387    -1.216364    -0.361396      22.30
 C      -2.929761     0.644023     0.143762      70.42
 H      -4.031473     0.799692     0.110394      21.81
 C      -2.383770     1.893607     0.521301       4.13
 O      -2.935844     3.145371     1.060456     117.30
 C      -4.503031     3.250721     1.391408      97.02
 H      -5.332501     3.115263     0.613703      25.85
 H      -5.092995     2.366071     1.988970      23.32
 H      -4.532726     4.449747     1.580283      23.12
 C      -0.967169     2.059447     0.430447      -2.86
 O      -0.278235     3.214751     0.779450     173.99
 C      -0.195978     0.847047    -0.027636      20.82
 H       0.864999     0.836489     0.167865      16.74
 C      -2.292597    -0.555669    -0.135343      33.56
 C      -3.325546    -1.612349    -0.626865      65.33
 H      -4.098118    -1.187281    -1.363400      19.35
 O      -2.770147    -2.523016    -1.758546     260.30
 H      -2.843883    -3.462070    -1.474254      21.10
 C      -3.977162    -2.368530     0.538314      84.92
 H      -3.114918    -2.758159     1.166093      18.93
 O      -4.957580    -1.366933     1.276986     227.31
 H      -4.446459    -0.891933     2.198213      20.66
 C      -5.030425    -3.387272     0.147330      93.35
 O      -4.507969    -4.742180    -0.220418     305.41
 H      -3.807935    -5.034711     0.426599      28.76
 H      -5.485651    -3.044606    -0.782270      26.98
 H      -5.482175    -3.652491     1.036420      26.31
55
name = lig-etoh-frame_380
 C       2.254996     1.941422    -2.271753      69.67
 H       1.585355     2.579889    -2.889517      20.11
 C       3.533389     1.555289    -0.254927      72.28
 H       4.021879     1.769182     0.757446      20.42
 C       4.077686     0.345490    -0.815397      24.79
 O       4.900102    -0.467062     0.025076     217.86
 C       4.826447    -0.215066     1.499540     104.74
 H       3.790961     0.023515     1.827819      23.87
 H       5.530591     0.625448     1.599694      25.47
 H       5.016396    -1.143516     1.946411      26.01
 C       3.609677    -0.093788    -2.143303      37.47
 O       3.809132    -1.449472    -2.293815     145.42
 H       4.653988    -1.540359    -1.587190      20.65
 C       2.741766     0.718601    -2.788669      58.59
 H       2.142002     0.212185    -3.716062      22.14
 C       2.663606     2.271478    -0.973211      27.85
 C       2.173438     3.659523    -0.386554      90.20
 H       2.320775     4.432197    -1.369134      19.96
 O       2.698521     3.961885     0.923111     312.32
 H       3.603396     3.921181     0.754225      30.28
 C       0.523742     3.929604    -0.276968      62.01
 H       0.192631     3.593584    -1.269633      19.05
 C       0.167495     5.366499    -0.058805      90.51
 O       0.735502     6.265131    -1.181145     167.88
 H       0.080966     5.642101    -1.919497      21.57
 H       0.509664     5.627977     1.110613      22.33
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 H      -0.977346     5.474138     0.093936      22.81
 C      -0.869401    -0.429796    -0.240893      39.48
 H      -0.271727    -1.558400    -0.083923      19.57
 C      -2.945440     0.686067     0.158912      57.14
 H      -4.003900     0.730049     0.001352      21.44
 C      -2.340009     1.905423     0.489148      -6.76
 O      -3.040722     3.142585     1.022490     130.92
 C      -4.573736     3.264213     1.385954     117.32
 H      -5.297472     3.106260     0.575558      27.04
 H      -4.828733     2.597039     2.139836      28.09
 H      -4.760346     4.239871     1.750125      26.97
 C      -0.904198     2.084786     0.374889       4.97
 O      -0.251066     3.189494     0.790544     168.17
 C      -0.199396     0.832581     0.006528      14.94
 H       0.878670     0.768721     0.298229      17.67
 C      -2.236975    -0.539521    -0.134590      13.93
 C      -3.320182    -1.650096    -0.641618      60.98
 H      -3.995579    -0.917083    -1.064968      21.22
 O      -2.785110    -2.572460    -1.811456     242.54
 H      -2.935701    -3.427544    -1.375562      20.30
 C      -3.994509    -2.362577     0.557447      83.44
 H      -3.228159    -3.042311     1.016648      16.58
 O      -4.989934    -1.342536     1.288139     232.29
 H      -4.708976    -0.897252     2.054910      25.72
 C      -5.038672    -3.415487     0.155361      63.93
 O      -4.510094    -4.798024    -0.240902     248.50
 H      -4.028779    -4.991617     0.668420      27.00
 H      -5.800633    -2.974525    -0.551287      26.69
 H      -5.470310    -3.367592     1.342349      23.85
55
name = lig-etoh-frame_381
 C       2.312113     1.840036    -2.243204      87.99
 H       1.726679     2.648506    -2.653695      22.50
 C       3.541099     1.537435    -0.268422      71.45
 H       3.814444     1.873134     0.667574      21.99
 C       4.080114     0.401950    -0.805565      -2.13
 O       4.864662    -0.527697     0.017233     221.30
 C       4.845813    -0.182381     1.494110      96.16
 H       3.795895     0.026318     1.710686      25.22
 H       5.506442     0.689620     1.527293      25.86
 H       5.213322    -1.202475     1.937736      24.32
 C       3.581882    -0.036191    -2.043311      23.89
 O       3.803248    -1.476911    -2.274984     173.25
 H       4.698076    -1.606577    -1.735089      22.02
 C       2.719860     0.702257    -2.901276      45.03
 H       2.131904     0.213160    -3.559579      24.56
 C       2.625476     2.334738    -0.967453      21.70
 C       2.137423     3.739033    -0.339308     102.02
 H       2.319387     4.397536    -1.242932      20.92
 O       2.714360     3.940803     0.886360     266.37
 H       3.809371     3.952424     0.904892      25.96
 C       0.620715     3.980386    -0.219483      74.64
 H       0.068239     3.508333    -1.052270      20.33
 C       0.162997     5.364252    -0.045724     120.06
 O       0.733973     6.191614    -1.114569     239.63
 H       0.448931     5.975845    -1.968438      30.51
 H       0.627200     5.700677     0.824334      25.93
 H      -0.893769     5.393443    -0.162989      25.51
 C      -0.799703    -0.488977    -0.211680      55.00
 H      -0.289958    -1.292958    -0.102508      24.24
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 C      -2.966873     0.739477     0.169751      39.78
 H      -4.074108     0.600822     0.007164      19.09
 C      -2.306692     1.976036     0.483229     -16.39
 O      -3.160112     3.122549     0.970409     140.23
 C      -4.606281     3.237149     1.366786      89.97
 H      -5.106816     3.058008     0.351322      22.93
 H      -4.508346     2.671717     2.445784      21.83
 H      -4.766317     4.264616     1.920097      23.85
 C      -0.857398     2.014481     0.307735      15.43
 O      -0.202116     3.182160     0.796971     150.71
 C      -0.225812     0.814599     0.074713      32.50
 H       0.915912     0.779240     0.245750      18.82
 C      -2.246173    -0.498138    -0.167558      -1.13
 C      -3.265654    -1.646077    -0.666300      59.21
 H      -4.058765    -0.896673    -0.932739      20.84
 O      -2.817949    -2.598315    -1.813054     196.74
 H      -3.060646    -3.593074    -1.347501      16.15
 C      -4.029693    -2.350861     0.551591      95.25
 H      -3.370222    -2.914886     1.230255      19.36
 O      -4.996509    -1.350126     1.261457     257.05
 H      -4.603371    -0.980163     2.144674      24.46
 C      -5.074058    -3.455144     0.212534     101.86
 O      -4.527484    -4.805960    -0.244376     284.11
 H      -4.159322    -5.109869     0.584920      30.30
 H      -5.995637    -3.161423    -0.288687      28.50
 H      -5.623987    -3.454557     1.078576      29.02
55
name = lig-etoh-frame_382
 C       2.318807     1.843713    -2.224797      65.86
 H       1.649613     2.541166    -2.810467      23.78
 C       3.553672     1.560602    -0.247429      59.39
 H       3.698443     2.007783     0.798570      18.07
 C       4.092942     0.426148    -0.767538       6.85
 O       4.813442    -0.573050    -0.004824     232.92
 C       4.874190    -0.180165     1.434371     107.73
 H       3.826943     0.041760     1.783428      25.31
 H       5.495278     0.716592     1.750316      26.77
 H       5.393608    -0.925547     1.959340      28.14
 C       3.564558    -0.079180    -1.960331      15.37
 O       3.815923    -1.464611    -2.263910     210.47
 H       4.585331    -1.834825    -1.923255      27.00
 C       2.719916     0.663269    -2.943603      39.16
 H       2.086231     0.150053    -3.814015      20.92
 C       2.596898     2.393115    -0.958065      31.58
 C       2.089173     3.748230    -0.343749     113.47
 H       2.572751     4.713658    -1.000642      18.00
 O       2.765198     3.939240     0.885764     308.49
 H       3.722917     4.026601     0.936192      30.59
 C       0.668456     3.934842    -0.187350      80.29
 H       0.240566     3.613797    -1.150586      20.68
 C       0.167676     5.387618    -0.070035      99.48
 O       0.746863     6.146610    -1.037859     225.01
 H       0.676455     6.125964    -2.085137      25.20
 H       0.688574     6.056910     0.875710      21.04
 H      -0.965459     5.356755    -0.189511      23.58
 C      -0.798773    -0.474695    -0.151241      37.86
 H       0.023210    -1.465973    -0.250611      19.47
 C      -2.964019     0.770628     0.158086      37.19
 H      -4.031011     0.700237     0.206330      20.47
 C      -2.350075     2.038951     0.487065     -12.95
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 O      -3.213914     3.113100     0.898310     184.98
 C      -4.571247     3.176781     1.386705     118.82
 H      -5.200439     2.928018     0.573927      27.05
 H      -4.702098     2.524446     2.180352      27.98
 H      -4.589119     4.273625     1.624620      25.22
 C      -0.862039     1.985193     0.289445      -2.80
 O      -0.136604     3.165576     0.815077     144.09
 C      -0.205675     0.744921     0.138971      46.54
 H       0.827583     0.864111     0.138652      20.86
 C      -2.261844    -0.449584    -0.222278      19.86
 C      -3.218237    -1.614247    -0.670464      72.28
 H      -4.129109    -1.221839    -1.194391      21.21
 O      -2.870233    -2.618708    -1.757458     293.25
 H      -3.104297    -3.454646    -1.545157      25.88
 C      -4.086036    -2.347334     0.548814      82.67
 H      -3.456666    -2.505057     1.501235      18.69
 O      -4.975398    -1.362294     1.220464     268.71
 H      -4.356663    -1.320798     2.153171      20.88
 C      -5.122679    -3.508679     0.260834      82.04
 O      -4.573243    -4.770120    -0.251275     267.70
 H      -4.052530    -5.292247     0.463629      26.03
 H      -5.951109    -3.313606    -0.515115      25.72
 H      -5.763897    -3.901172     1.279007      24.36
55
name = lig-etoh-frame_383
 C       2.260941     1.912775    -2.277076      68.72
 H       1.564929     2.300550    -2.995844      22.33
 C       3.533192     1.670150    -0.184524      80.63
 H       3.781917     1.905564     0.823133      18.15
 C       4.097922     0.403018    -0.717789       8.63
 O       4.766262    -0.585320    -0.006934     244.05
 C       4.906965    -0.166967     1.373748     112.38
 H       3.950245    -0.091809     1.901379      25.42
 H       5.413141     0.758314     1.647091      28.20
 H       5.498900    -0.944443     1.999402      26.10
 C       3.541864    -0.182363    -1.963624      23.93
 O       3.813990    -1.423736    -2.267601     154.68
 H       4.660418    -2.092751    -1.955969      21.40
 C       2.739159     0.606712    -2.867502      49.03
 H       2.404160     0.330011    -3.859280      21.13
 C       2.613649     2.396188    -0.962002      32.63
 C       2.158939     3.746323    -0.362781     119.94
 H       2.495043     4.689083    -0.887639      19.86
 O       2.801917     3.945350     0.936848     284.68
 H       3.780417     4.093383     0.751183      30.07
 C       0.621567     3.879665    -0.184277      71.07
 H       0.430823     3.745087    -1.294920      18.77
 C       0.170762     5.415158    -0.059224     114.79
 O       0.807102     6.181958    -1.009605     252.00
 H       0.506089     5.800789    -1.973617      26.89
 H       0.313414     5.914600     0.844503      25.83
 H      -0.913615     5.384049     0.019736      25.35
 C      -0.823736    -0.492981    -0.091729      54.52
 H      -0.259053    -1.219181    -0.443072      21.66
 C      -2.942279     0.792597     0.137520      49.78
 H      -4.034852     0.802362     0.375050      19.94
 C      -2.409788     2.042683     0.479830       8.46
 O      -3.187271     3.112025     0.808288     204.96
 C      -4.514371     3.104647     1.378390     119.06
 H      -5.505057     2.817555     0.745438      24.64
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 H      -4.961524     2.263262     2.169840      22.77
 H      -4.581731     4.205112     1.450252      24.71
 C      -0.917512     2.019971     0.343410     -10.47
 O      -0.065950     3.120085     0.823249     164.74
 C      -0.178148     0.702693     0.196095      14.49
 H       0.997973     0.904934     0.047439      15.83
 C      -2.268619    -0.416555    -0.279170      23.86
 C      -3.251657    -1.613140    -0.676139      74.72
 H      -4.030958    -1.264467    -1.358535      20.59
 O      -2.891128    -2.608489    -1.695576     263.94
 H      -3.260279    -3.573732    -1.468911      20.02
 C      -4.138396    -2.339971     0.584452      89.59
 H      -3.373975    -2.529734     1.303934      22.57
 O      -4.931603    -1.364351     1.196526     359.28
 H      -4.600922    -1.358916     1.999645      32.48
 C      -5.186427    -3.609221     0.320167      99.39
 O      -4.616944    -4.740303    -0.275700     307.15
 H      -3.884174    -5.145608     0.310375      26.36
 H      -5.679328    -3.263061    -0.583261      26.13
 H      -5.566665    -3.910677     1.182749      28.57
55
name = lig-etoh-frame_384
 C       2.219842     1.926332    -2.352609      55.28
 H       1.441794     2.358078    -3.041999      17.60
 C       3.543987     1.700974    -0.153871      56.47
 H       3.875780     1.956463     0.853985      16.30
 C       4.021850     0.394878    -0.698233      15.98
 O       4.734010    -0.575618     0.020359     226.41
 C       4.955791    -0.179961     1.366340     115.90
 H       3.974991    -0.260165     1.931581      24.74
 H       5.400540     0.869399     1.260926      26.13
 H       5.543283    -0.982295     1.769334      26.39
 C       3.540550    -0.208078    -1.945854      21.54
 O       3.822817    -1.459284    -2.307657     213.51
 H       4.598774    -1.828685    -1.838407      24.60
 C       2.763269     0.613770    -2.708234      98.38
 H       2.690162     0.392344    -3.820483      28.75
 C       2.636456     2.402251    -1.004120      62.43
 C       2.245396     3.724927    -0.330364     106.86
 H       2.316089     4.682661    -1.154178      19.39
 O       2.839701     3.954983     0.997235     270.60
 H       3.841386     4.154389     0.650755      28.50
 C       0.577312     3.880950    -0.220000      57.97
 H       0.253210     3.611873    -1.243598      20.61
 C       0.160564     5.395439    -0.009656      90.32
 O       0.859537     6.233863    -1.030829     214.40
 H       0.427704     5.727376    -1.716454      30.92
 H       0.210392     5.713801     1.201005      23.39
 H      -1.000825     5.427607    -0.108147      24.12
 C      -0.905961    -0.474738    -0.059310      28.82
 H      -0.362876    -1.431595    -0.637656      17.38
 C      -2.954121     0.789702     0.116820      55.83
 H      -4.020520     0.706269     0.308231      19.91
 C      -2.388553     1.998027     0.453386      20.51
 O      -3.143742     3.118752     0.721174     210.42
 C      -4.526025     2.999464     1.348157     116.37
 H      -5.277332     2.843485     0.642756      26.95
 H      -4.577429     2.454758     2.251074      27.05
 H      -4.768173     4.107314     1.681948      25.42
 C      -0.955316     2.033006     0.446635      -0.82
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 O      -0.013738     3.053984     0.811976     176.24
 C      -0.164125     0.756207     0.240951      13.16
 H       0.832058     0.743277     0.126678      18.03
 C      -2.286961    -0.409894    -0.306005      17.01
 C      -3.359533    -1.623978    -0.691569      62.19
 H      -4.046803    -0.852015    -1.216574      21.25
 O      -2.871938    -2.623725    -1.635358     236.91
 H      -3.397683    -3.471663    -1.254657      18.74
 C      -4.145992    -2.351215     0.605532      77.18
 H      -3.202844    -2.888467     1.087482      20.18
 O      -4.914490    -1.339920     1.171422     285.11
 H      -4.827200    -1.213977     2.280956      23.93
 C      -5.180045    -3.649677     0.322150      71.99
 O      -4.622162    -4.752388    -0.319997     313.21
 H      -3.838964    -4.878428     0.218009      30.60
 H      -5.874378    -3.066882    -0.385016      26.19
 H      -5.755153    -3.767576     1.464703      25.83
55
name = lig-etoh-frame_385
 C       2.218991     1.904708    -2.360832       6.48
 H       1.526057     2.498619    -2.910628      17.81
 C       3.571574     1.633994    -0.195736      70.41
 H       3.868136     2.153927     0.765013      18.37
 C       3.905387     0.380836    -0.673358      24.04
 O       4.701119    -0.563043     0.038272     224.49
 C       5.005012    -0.194879     1.367926     119.76
 H       4.084848    -0.226356     1.939597      26.06
 H       5.431109     0.773619     1.244517      26.44
 H       5.806013    -0.949642     1.654647      25.91
 C       3.556594    -0.161397    -1.861374      18.76
 O       3.843448    -1.516446    -2.361263     196.53
 H       4.594147    -1.659220    -1.709510      22.62
 C       2.747131     0.681270    -2.615134      61.60
 H       2.834749     0.296124    -3.684938      26.31
 C       2.660110     2.424152    -1.050230     108.37
 C       2.243381     3.721814    -0.313787      98.00
 H       2.420246     4.507874    -1.091338      20.65
 O       2.884901     3.975654     1.010388     325.10
 H       3.797468     4.170451     0.999077      32.71
 C       0.571425     3.897142    -0.262024      46.19
 H       0.020184     3.427264    -1.116382      18.38
 C       0.124156     5.356809     0.080846     103.90
 O       0.887822     6.274116    -1.022496      81.54
 H       0.372054     5.860781    -1.966989      23.55
 H       0.421184     5.544228     1.002466      27.97
 H      -0.836794     5.484461    -0.365959      25.02
 C      -0.957897    -0.445751    -0.084176      44.31
 H      -0.502463    -1.373911    -0.380333      19.84
 C      -2.997250     0.745648     0.086532      52.68
 H      -4.080779     0.630582     0.097042      19.13
 C      -2.329585     1.959689     0.430233       8.52
 O      -3.115651     3.140629     0.652462     184.12
 C      -4.507366     2.950306     1.320196      87.45
 H      -5.123615     2.630986     0.350669      21.57
 H      -4.172183     2.383355     2.354738      22.06
 H      -4.793425     3.859873     1.819598      25.96
 C      -0.905671     1.983659     0.553528      24.24
 O       0.013244     2.999557     0.805257     175.09
 C      -0.257705     0.804859     0.270284      24.76
 H       0.940039     0.678381     0.291658      17.43
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 C      -2.342825    -0.429565    -0.283448      16.04
 C      -3.477557    -1.587694    -0.703586      67.63
 H      -4.182978    -0.863740    -1.040237      23.14
 O      -2.860336    -2.641581    -1.554575     259.53
 H      -3.338823    -3.362092    -1.333222      25.40
 C      -4.101135    -2.400263     0.588816      84.87
 H      -3.331691    -2.916262     1.097992      23.45
 O      -4.901501    -1.299945     1.186078     275.87
 H      -4.986951    -1.230344     2.235728      26.67
 C      -5.201275    -3.573713     0.340513     100.13
 O      -4.611053    -4.774864    -0.362028     305.94
 H      -3.718954    -4.864653     0.181093      28.11
 H      -6.143441    -3.206960    -0.078041      28.29
 H      -5.656275    -3.735213     1.203844      30.65
55
name = lig-etoh-frame_386
 C       2.238013     1.938384    -2.265187      41.54
 H       1.635612     2.580434    -2.942128      21.89
 C       3.553577     1.611202    -0.283059      64.54
 H       3.861041     2.090474     0.574915      18.63
 C       3.845234     0.315121    -0.580144      50.54
 O       4.664904    -0.559479     0.042512     254.05
 C       5.078588    -0.218623     1.367469     126.64
 H       4.236534    -0.169445     2.130398      26.67
 H       5.553944     0.833561     1.542015      26.64
 H       5.958433    -0.806214     1.688656      27.99
 C       3.525542    -0.131067    -1.835638      27.56
 O       3.881044    -1.510970    -2.385011     121.00
 H       4.655393    -1.808686    -1.603706      20.78
 C       2.741883     0.693216    -2.635824      46.65
 H       2.617133     0.254097    -3.600503      24.57
 C       2.699217     2.421332    -1.047600      87.79
 C       2.194315     3.718887    -0.322356      92.58
 H       2.764888     4.644774    -0.976859      17.39
 O       2.884179     3.991931     1.004731     283.41
 H       3.918575     4.216638     1.175940      25.76
 C       0.582772     3.880212    -0.274687      56.21
 H       0.061397     3.483885    -1.181459      20.71
 C       0.126418     5.303018     0.054701      83.33
 O       0.881765     6.285221    -1.010874     123.01
 H       0.603420     6.236850    -1.855487      30.45
 H       0.668020     5.665057     1.118960      23.66
 H      -0.947490     5.556025    -0.238527      24.62
 C      -1.001330    -0.396994    -0.115000      57.75
 H      -0.353422    -1.401544    -0.152577      20.94
 C      -3.046818     0.726736     0.056344      37.36
 H      -4.147655     0.796271    -0.115869      19.86
 C      -2.315535     1.943423     0.422059     -11.91
 O      -3.084816     3.168418     0.597181     176.54
 C      -4.416184     2.886131     1.285744     101.73
 H      -5.038500     2.348677     0.650716      26.49
 H      -4.157874     2.073248     1.946206      26.51
 H      -4.873571     3.892931     1.739750      24.59
 C      -0.842349     1.937099     0.629978      19.82
 O       0.032919     2.978443     0.833894     174.93
 C      -0.330389     0.736741     0.277496      46.70
 H       0.681677     0.775406     0.494813      20.68
 C      -2.434955    -0.477219    -0.238518      23.43
 C      -3.526342    -1.573054    -0.665630      63.39
 H      -4.532033    -1.176280    -1.203663      21.78
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 O      -2.850800    -2.621313    -1.479138     181.70
 H      -3.438902    -3.582829    -1.494612      17.22
 C      -4.105651    -2.412839     0.543083      79.82
 H      -3.326005    -2.751391     1.351902      19.97
 O      -4.890270    -1.268644     1.211528     270.15
 H      -4.879089    -1.389622     2.102644      31.73
 C      -5.203302    -3.467409     0.323458      78.05
 O      -4.595747    -4.768606    -0.386184     251.89
 H      -3.808074    -5.074724     0.113855      26.93
 H      -6.215785    -3.375185    -0.186642      26.17
 H      -5.449455    -4.000788     1.496973      25.30
55
name = lig-etoh-frame_387
 C       2.256871     1.990103    -2.182361      55.07
 H       1.728763     2.536096    -2.940323      23.74
 C       3.528771     1.619822    -0.329515      65.47
 H       3.978274     1.994428     0.673362      17.85
 C       3.808627     0.240315    -0.514497      35.42
 O       4.660404    -0.575248     0.090102     244.24
 C       5.174955    -0.199207     1.409317     130.42
 H       4.440178    -0.326198     2.204314      28.21
 H       5.533767     0.788137     1.549184      28.35
 H       5.959679    -0.910960     1.687926      28.21
 C       3.466647    -0.170054    -1.881518      23.60
 O       3.935753    -1.445940    -2.356470     222.78
 H       4.462701    -1.960404    -1.885101      27.93
 C       2.737705     0.671949    -2.707310      52.02
 H       2.171223     0.269640    -3.685212      21.24
 C       2.713566     2.435779    -0.996519      42.93
 C       2.214154     3.752894    -0.352549     101.82
 H       2.615824     4.603019    -0.855020      22.04
 O       2.842956     3.996417     1.013968     276.78
 H       3.824377     4.191021     0.823203      27.96
 C       0.605069     3.839078    -0.268558      64.99
 H       0.302082     3.623680    -1.301353      22.52
 C       0.176848     5.304851    -0.022049     106.43
 O       0.877853     6.292104    -0.944503     146.02
 H       0.536084     6.325175    -1.973975      25.36
 H       0.520078     5.692820     0.829969      28.27
 H      -0.898948     5.433607     0.218353      26.40
 C      -1.063245    -0.444122    -0.153206      56.07
 H      -0.303569    -1.273015     0.033242      22.00
 C      -3.091413     0.776043     0.028876      32.09
 H      -4.088873     1.013961    -0.248321      20.91
 C      -2.321505     1.952463     0.425159      -8.35
 O      -3.053147     3.178411     0.550404     195.72
 C      -4.295847     2.822062     1.244589     104.41
 H      -5.211754     2.224912     0.698534      24.63
 H      -4.177835     1.847609     1.960677      23.21
 H      -4.757314     3.684881     1.531430      27.20
 C      -0.873155     1.927920     0.650352      11.64
 O       0.055223     2.984091     0.886855     159.93
 C      -0.360283     0.638439     0.299134      25.18
 H       0.771667     0.617935     0.569232      19.89
 C      -2.540472    -0.519921    -0.203642      20.70
 C      -3.549182    -1.630598    -0.629009      94.27
 H      -4.370008    -1.451570    -1.242183      23.45
 O      -2.842725    -2.610485    -1.423296     275.88
 H      -3.422649    -3.370386    -1.554002      22.75
 C      -4.147508    -2.348127     0.536276      98.30
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 H      -3.413469    -2.573136     1.284819      21.19
 O      -4.885874    -1.245814     1.224215     236.76
 H      -4.638323    -1.618120     2.287136      23.09
 C      -5.175468    -3.473612     0.351627     107.82
 O      -4.593149    -4.733820    -0.416833     295.68
 H      -3.956317    -5.162839     0.198401      27.20
 H      -5.999409    -3.298874    -0.310366      28.43
 H      -5.202083    -3.840819     1.226093      32.28
55
name = lig-etoh-frame_388
 C       2.285806     1.969013    -2.196427      39.45
 H       1.654124     2.593381    -2.853650      22.73
 C       3.575152     1.573776    -0.239179      63.27
 H       3.979549     1.923821     0.652529      20.57
 C       3.745201     0.222034    -0.563379      21.67
 O       4.689170    -0.611170     0.180848     210.43
 C       5.264838    -0.197264     1.472390     113.91
 H       4.479099    -0.492993     2.233893      26.04
 H       5.609052     0.894674     1.360912      24.93
 H       6.025193    -1.055877     1.544523      25.77
 C       3.430262    -0.255975    -1.902152      25.12
 O       3.960141    -1.352619    -2.358610     181.79
 H       4.481075    -2.100557    -1.803998      21.65
 C       2.673094     0.678579    -2.779290      50.72
 H       2.101098     0.397635    -3.556014      24.12
 C       2.688791     2.501987    -0.935604      40.93
 C       2.246705     3.769766    -0.331039      92.97
 H       2.313396     4.839893    -1.101193      18.82
 O       2.783651     3.993025     0.998036     310.97
 H       3.657231     4.172302     0.690433      29.54
 C       0.656110     3.810259    -0.256144      55.73
 H       0.390673     3.516412    -1.332340      20.43
 C       0.230535     5.331197    -0.101742     103.59
 O       0.852266     6.298117    -0.888955     193.51
 H       0.359984     6.103267    -1.794662      26.87
 H       0.687004     5.706804     1.006971      23.48
 H      -0.829013     5.258104     0.287917      24.72
 C      -1.151827    -0.555868    -0.154754      29.75
 H      -0.509650    -1.492078    -0.099195      22.18
 C      -3.098392     0.841193    -0.003458      29.00
 H      -4.131726     1.124373    -0.347419      21.08
 C      -2.310105     1.974720     0.419409       8.12
 O      -3.030576     3.154580     0.514769     230.72
 C      -4.220170     2.702401     1.192260     115.31
 H      -5.010234     2.490620     0.537318      26.25
 H      -4.062443     2.165273     2.167188      24.93
 H      -4.661037     3.751240     1.626416      24.99
 C      -0.936667     1.905881     0.610618      12.07
 O       0.064900     2.998819     0.926398     126.55
 C      -0.352057     0.602099     0.353648      21.02
 H       0.704261     0.254172     0.437829      21.22
 C      -2.625573    -0.505271    -0.186716      14.18
 C      -3.526810    -1.717352    -0.614029      78.63
 H      -4.352587    -1.186873    -1.358908      21.71
 O      -2.803078    -2.605852    -1.391004     269.19
 H      -3.456247    -3.338860    -1.500657      21.21
 C      -4.207106    -2.247135     0.565963     105.80
 H      -3.301299    -2.667351     1.159437      20.50
 O      -4.887838    -1.250219     1.277874     338.36
 H      -4.558630    -1.348484     2.182894      28.75
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 C      -5.083089    -3.524815     0.314324      69.57
 O      -4.596846    -4.676246    -0.447931     284.53
 H      -4.078403    -5.143204     0.333040      24.76
 H      -5.964042    -3.060330    -0.265073      27.21
 H      -5.419768    -3.853486     1.567581      26.20
55
name = lig-etoh-frame_389
 C       2.311787     1.939171    -2.237819       6.33
 H       1.575827     2.591909    -2.718332      20.56
 C       3.586881     1.543086    -0.129750      70.77
 H       4.047673     1.903622     0.846703      18.99
 C       3.725119     0.218982    -0.626955       8.08
 O       4.701283    -0.651091     0.248071     194.37
 C       5.332277    -0.228310     1.503620     122.12
 H       4.619140    -0.346956     2.317861      26.99
 H       5.721414     0.764878     1.398480      27.18
 H       6.184810    -0.860223     1.518409      27.78
 C       3.368675    -0.256723    -1.888174      32.40
 O       3.998642    -1.325889    -2.411670     179.89
 H       4.380145    -1.852449    -1.527332      20.51
 C       2.613995     0.697993    -2.754741      56.18
 H       2.072814     0.355649    -3.797133      21.75
 C       2.710997     2.487838    -0.902598      59.91
 C       2.214108     3.809934    -0.310271     112.88
 H       2.270378     4.647403    -1.027564      23.23
 O       2.723204     3.996254     0.957096     277.38
 H       3.811300     4.266038     0.980590      25.04
 C       0.715887     3.796925    -0.255570      59.84
 H       0.281066     3.275860    -1.091239      21.59
 C       0.298438     5.327021    -0.019568     113.53
 O       0.789274     6.300368    -0.885444     232.37
 H       0.408177     6.071066    -1.722214      30.69
 H       0.751968     5.407729     0.881885      26.89
 H      -0.824352     5.345523    -0.125408      24.72
 C      -1.240241    -0.637345    -0.084915      28.77
 H      -0.973489    -1.757647    -0.460334      18.54
 C      -3.090972     0.877207    -0.055489      39.44
 H      -4.088931     1.043076    -0.350603      23.47
 C      -2.300505     1.977738     0.377829      11.35
 O      -3.004650     3.119854     0.493319     239.15
 C      -4.199077     2.719085     1.193138     111.94
 H      -4.928704     2.461779     0.319411      23.23
 H      -3.946754     2.197777     2.190515      24.10
 H      -4.461007     3.594801     1.648225      27.19
 C      -0.909374     1.862053     0.548523      10.05
 O       0.047828     3.009541     0.933487     126.44
 C      -0.387423     0.521271     0.377391      33.37
 H       0.654482     0.239112     0.385255      21.32
 C      -2.647437    -0.449705    -0.190159      21.27
 C      -3.523274    -1.673331    -0.657363      91.91
 H      -4.170059    -1.081464    -1.198971      24.47
 O      -2.747285    -2.629477    -1.375112     218.93
 H      -3.388275    -3.544009    -1.446744      16.39
 C      -4.207173    -2.227896     0.635281     113.69
 H      -3.321479    -2.688775     1.078557      23.39
 O      -4.907148    -1.246423     1.340048     357.79
 H      -4.472827    -1.068013     2.259552      27.67
 C      -5.053266    -3.549456     0.322912     128.03
 O      -4.595589    -4.609562    -0.451934     331.76
 H      -4.064408    -5.103552     0.167645      30.82
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 H      -5.930938    -3.090966    -0.081192      29.41
 H      -5.574478    -3.768602     1.108815      30.76
55
name = lig-etoh-frame_390
 C       2.318346     1.963535    -2.218593      41.18
 H       1.573488     2.551158    -2.755848      18.85
 C       3.536420     1.553029    -0.057168      43.49
 H       4.007555     1.760174     0.907767      20.41
 C       3.776469     0.240119    -0.599593       1.32
 O       4.683312    -0.696354     0.268908     176.83
 C       5.379275    -0.257251     1.493268     113.62
 H       4.812758    -0.185073     2.477836      26.28
 H       5.810093     0.813052     1.498271      26.43
 H       6.412000    -0.792436     1.657130      26.01
 C       3.296644    -0.186270    -1.898230      20.93
 O       4.037808    -1.338781    -2.449989     209.90
 H       4.348808    -1.600601    -1.662044      27.68
 C       2.554228     0.668028    -2.715001      54.24
 H       2.386716     0.390483    -3.672418      28.51
 C       2.784726     2.380703    -0.896145      52.31
 C       2.181466     3.775511    -0.312778     110.71
 H       2.594096     4.691623    -1.130933      21.26
 O       2.705444     4.027965     0.955294     347.21
 H       3.546532     4.265277     1.198821      31.04
 C       0.712106     3.783305    -0.238748      61.68
 H       0.161033     3.175936    -1.026968      20.67
 C       0.306031     5.257626     0.068355      96.48
 O       0.740410     6.318183    -0.904516     131.07
 H       0.466158     6.060345    -1.975144      23.77
 H       0.756346     5.406243     1.193862      23.55
 H      -0.723700     5.426621    -0.234389      23.07
 C      -1.319307    -0.689405     0.007727      54.31
 H      -1.130938    -1.608165    -0.471988      18.73
 C      -3.076433     0.874761    -0.118217      41.64
 H      -4.163382     0.993078    -0.341749      20.75
 C      -2.272960     1.946266     0.297601       0.63
 O      -2.969671     3.109998     0.488347     213.80
 C      -4.205766     2.807902     1.209830      93.07
 H      -4.940372     2.279009     0.592110      25.50
 H      -3.978646     1.836484     1.857641      24.95
 H      -4.577556     3.832890     1.691685      24.11
 C      -0.816380     1.807412     0.489524      -0.45
 O       0.009591     2.998034     0.919481     136.12
 C      -0.451912     0.390644     0.361149      32.77
 H       0.734972     0.430680     0.417588      19.27
 C      -2.615255    -0.403430    -0.213212      35.76
 C      -3.515829    -1.554169    -0.669484      55.56
 H      -4.401536    -1.119015    -1.413640      20.71
 O      -2.704935    -2.678772    -1.369647     226.08
 H      -3.119017    -3.458793    -1.309907      22.97
 C      -4.147077    -2.280598     0.679581      86.42
 H      -3.282579    -2.583218     1.352126      21.41
 O      -4.945630    -1.247182     1.417676     274.94
 H      -4.255284    -0.786704     2.206858      22.68
 C      -5.091504    -3.476261     0.328430      84.03
 O      -4.577551    -4.555824    -0.466598     292.42
 H      -3.883629    -5.120832     0.004111      27.74
 H      -6.001096    -3.153509    -0.335914      25.28
 H      -5.743466    -4.042435     1.336749      23.99
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name = lig-etoh-frame_391
 C       2.310135     1.991197    -2.158154      70.99
 H       1.700963     2.640080    -2.809215      21.80
 C       3.488201     1.507087    -0.022115      47.64
 H       3.840106     1.791065     0.953291      21.08
 C       3.857916     0.272671    -0.509940      -2.07
 O       4.648201    -0.731462     0.266220     184.66
 C       5.449109    -0.242982     1.480363     115.13
 H       4.886822    -0.285993     2.420715      27.07
 H       5.732950     0.793952     1.321352      26.97
 H       6.248828    -0.893396     1.652276      27.73
 C       3.311838    -0.154908    -1.889335       7.44
 O       4.031162    -1.321786    -2.483434     101.46
 H       4.685523    -1.720574    -1.606142      19.40
 C       2.516449     0.650928    -2.650802      60.33
 H       2.533759     0.352001    -3.808014      24.55
 C       2.811019     2.315504    -0.908853      34.68
 C       2.254340     3.690242    -0.363718     100.01
 H       2.624710     4.482439    -0.964612      23.95
 O       2.659478     4.062434     1.001285     292.18
 H       3.664262     4.341444     1.095624      26.06
 C       0.636012     3.761011    -0.217461      66.72
 H       0.252099     3.490470    -1.188196      22.56
 C       0.279993     5.192487     0.119961      94.61
 O       0.718364     6.331816    -0.941088     201.88
 H       0.480046     5.974751    -1.744820      32.74
 H       0.493257     5.634278     1.065074      25.30
 H      -0.859705     5.258728     0.204752      24.31
 C      -1.329867    -0.707470     0.108107      52.80
 H      -0.797635    -1.759737    -0.320337      17.52
 C      -3.085454     0.878976    -0.183434      43.61
 H      -4.140941     1.055455    -0.337223      20.86
 C      -2.214938     1.920067     0.208772      -4.87
 O      -2.936139     3.124499     0.495808     186.08
 C      -4.219104     2.888978     1.240685     104.53
 H      -5.136006     2.408704     0.703117      25.22
 H      -4.045071     1.923596     1.793359      25.82
 H      -4.632217     3.737238     1.666487      26.65
 C      -0.773882     1.743399     0.434697       2.15
 O      -0.034503     2.945088     0.892931     173.73
 C      -0.445338     0.324970     0.343072      44.21
 H       0.559382     0.223328     0.446864      22.30
 C      -2.622607    -0.399267    -0.269720      39.31
 C      -3.536131    -1.483371    -0.674953      76.28
 H      -4.305835    -1.409510    -1.328025      23.88
 O      -2.655859    -2.672594    -1.366678     120.87
 H      -3.192762    -3.599240    -1.069426      13.93
 C      -4.091166    -2.306468     0.713852      80.11
 H      -3.335920    -2.501748     1.508639      21.35
 O      -4.962745    -1.248644     1.498113     337.65
 H      -4.339852    -0.879669     1.951740      31.06
 C      -5.201636    -3.419484     0.367408      97.31
 O      -4.541164    -4.515300    -0.496389     290.92
 H      -3.762765    -4.964165     0.022740      26.12
 H      -5.834404    -3.117101    -0.417817      27.57
 H      -5.425350    -3.874649     1.179886      29.78
55
name = lig-etoh-frame_392
 C       2.291568     1.974697    -2.128099      67.10
 H       1.904555     2.794180    -2.733897      21.21
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 C       3.469453     1.429025     0.015394      49.90
 H       3.575408     1.974744     1.028050      19.66
 C       3.930668     0.239020    -0.442127      16.07
 O       4.610397    -0.741017     0.255924     206.62
 C       5.478176    -0.225036     1.437782      98.08
 H       4.765464    -0.389691     2.286622      24.94
 H       5.784930     0.792958     1.116536      25.26
 H       6.249171    -1.108911     1.474040      24.54
 C       3.438438    -0.185982    -1.817297       5.94
 O       4.007606    -1.283579    -2.468682     186.52
 H       4.739110    -1.731974    -2.057330      25.07
 C       2.510709     0.654214    -2.617360      53.44
 H       2.437616     0.418016    -3.653691      25.36
 C       2.773510     2.336452    -0.899317      39.39
 C       2.318156     3.568781    -0.355691      71.76
 H       2.592291     4.618060    -1.115082      18.97
 O       2.635077     4.091645     1.059701     253.88
 H       3.624978     4.345725     0.793885      24.52
 C       0.587284     3.740744    -0.208487      39.72
 H       0.250484     3.784924    -1.309837      18.90
 C       0.187967     5.200236     0.134308      80.85
 O       0.692246     6.306698    -0.930358     127.38
 H       0.330500     5.821933    -1.841069      25.37
 H       0.599097     5.759854     1.058123      23.21
 H      -0.856489     5.047448     0.450261      24.29
 C      -1.276799    -0.755749     0.165134      31.28
 H      -0.781856    -1.620152     0.152326      19.48
 C      -3.087330     0.905177    -0.246389      42.48
 H      -4.126041     1.182333    -0.406959      18.48
 C      -2.177567     1.922296     0.139505       2.24
 O      -2.905707     3.148278     0.509781     162.26
 C      -4.235237     2.910636     1.233394      87.93
 H      -5.125811     2.861692     0.549897      23.70
 H      -4.053125     2.194667     2.222944      23.18
 H      -4.515586     3.881514     1.843526      25.50
 C      -0.805393     1.692991     0.380581      20.62
 O      -0.069230     2.855727     0.832422     179.01
 C      -0.389027     0.341022     0.345646      36.92
 H       0.685983    -0.231705     0.533299      18.34
 C      -2.649568    -0.432720    -0.342504      26.31
 C      -3.521122    -1.555813    -0.631695      67.07
 H      -4.471081    -1.440798    -1.386121      21.27
 O      -2.627084    -2.651688    -1.351964     166.95
 H      -3.223061    -3.376132    -0.999605      17.18
 C      -4.111161    -2.260145     0.732065      89.81
 H      -3.312161    -2.648336     1.378210      23.28
 O      -4.982780    -1.282393     1.539446     281.83
 H      -4.170279    -0.762754     2.125632      23.29
 C      -5.201026    -3.366963     0.352362      63.89
 O      -4.491400    -4.475801    -0.516767     302.96
 H      -3.879379    -4.763718     0.145152      28.86
 H      -6.014488    -2.870869    -0.310510      26.22
 H      -5.519927    -3.851294     1.519978      25.50
55
name = lig-etoh-frame_393
 C       2.279616     1.937471    -2.133355      71.04
 H       1.959222     2.799584    -2.732196      21.68
 C       3.429699     1.424762     0.052262      34.29
 H       3.467147     1.834367     1.001117      22.41
 C       3.961129     0.155232    -0.438524      32.46
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 O       4.597654    -0.748362     0.256430     247.27
 C       5.467946    -0.263635     1.349743     111.13
 H       4.791133    -0.234430     2.222286      25.67
 H       5.954042     0.723006     1.146710      26.64
 H       6.244932    -0.968025     1.336254      27.06
 C       3.575445    -0.190292    -1.737458      30.73
 O       3.965041    -1.244978    -2.469287     193.85
 H       4.803604    -1.732972    -2.194978      24.44
 C       2.574499     0.647484    -2.542150      51.70
 H       2.237881     0.384302    -3.615206      24.01
 C       2.755470     2.310835    -0.828769      35.76
 C       2.269784     3.580349    -0.295263      92.58
 H       2.466150     4.346328    -1.016530      22.15
 O       2.653119     4.098586     1.066325     319.31
 H       3.515485     4.396171     0.989756      29.43
 C       0.589663     3.745127    -0.227299      41.63
 H       0.117809     3.605222    -1.184259      21.44
 C       0.120141     5.260774     0.174280      86.94
 O       0.624764     6.216257    -0.911037     173.12
 H       0.233091     5.989591    -1.862648      25.89
 H       0.881071     5.556161     0.954951      23.05
 H      -0.994534     5.111779     0.338903      23.78
 C      -1.261715    -0.727620     0.171758      20.78
 H      -0.883919    -1.879603     0.643130      17.65
 C      -3.064296     0.909705    -0.318882      50.60
 H      -4.111058     1.238849    -0.550922      18.27
 C      -2.212714     1.939698     0.096746       7.98
 O      -2.871298     3.164550     0.530043     180.21
 C      -4.227760     2.981155     1.264469     100.43
 H      -4.981687     3.006027     0.453679      24.17
 H      -4.205315     2.360304     2.164676      26.34
 H      -4.132814     3.931841     1.747020      27.02
 C      -0.838466     1.678205     0.331876      18.32
 O      -0.085495     2.758605     0.738599     190.78
 C      -0.300811     0.316983     0.367067      39.64
 H       0.602698    -0.031695     0.620520      21.29
 C      -2.624073    -0.463484    -0.375915      32.72
 C      -3.525900    -1.700070    -0.608183      97.88
 H      -4.302366    -1.307177    -1.167602      26.49
 O      -2.626287    -2.604892    -1.315630     215.82
 H      -3.176455    -3.475801    -1.183807      15.94
 C      -4.188800    -2.190083     0.734388     100.06
 H      -3.310187    -2.802762     1.154697      21.29
 O      -4.952466    -1.320801     1.563935     355.89
 H      -4.413752    -0.834183     2.326640      27.22
 C      -5.159994    -3.329736     0.360228     108.17
 O      -4.463947    -4.406860    -0.507586     308.62
 H      -3.915876    -4.801513     0.313617      26.89
 H      -6.068132    -2.870596     0.036388      29.60
 H      -5.631995    -3.654933     1.146540      31.13
55
name = lig-etoh-frame_394
 C       2.304264     1.909290    -2.109111      65.76
 H       1.786148     2.577938    -2.824744      18.67
 C       3.392588     1.414984     0.057015      47.84
 H       3.560065     1.583028     1.203207      19.98
 C       3.920704     0.146904    -0.458939      42.21
 O       4.629333    -0.788867     0.284243     276.08
 C       5.446486    -0.299110     1.253525     122.50
 H       4.990763    -0.088448     2.266016      26.49
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 H       5.970457     0.660284     1.130597      27.46
 H       6.354111    -1.016182     1.413998      26.05
 C       3.637421    -0.140551    -1.724803      43.32
 O       3.930940    -1.245285    -2.486743     155.16
 H       4.896502    -1.743408    -2.151873      21.23
 C       2.686923     0.632828    -2.464743      55.16
 H       2.155739     0.179436    -3.354558      23.08
 C       2.732195     2.247998    -0.737433      55.55
 C       2.128380     3.651484    -0.182516      87.22
 H       2.497781     4.411246    -1.190789      22.15
 O       2.671978     4.085188     1.050389     285.04
 H       3.642246     4.486824     1.256862      24.43
 C       0.586691     3.749197    -0.240795      54.32
 H       0.111344     3.303408    -1.169689      19.19
 C       0.112709     5.283925     0.176633     107.38
 O       0.535163     6.120095    -0.883139     262.76
 H       0.140697     5.958733    -1.742049      28.99
 H       0.783081     5.424823     1.033489      25.37
 H      -0.962945     5.444356     0.247084      25.43
 C      -1.257584    -0.715530     0.182224      46.27
 H      -1.245276    -1.567947     0.629422      20.82
 C      -3.041694     0.872530    -0.408320      52.88
 H      -4.042695     1.092461    -0.708149      24.09
 C      -2.280681     1.952362     0.078843       2.83
 O      -2.826039     3.156692     0.549825     196.00
 C      -4.155171     3.112581     1.275818      93.50
 H      -4.990374     2.978707     0.473944      24.88
 H      -4.450769     2.092301     1.970046      22.67
 H      -4.045362     4.156260     1.627417      24.45
 C      -0.848766     1.666551     0.280661       9.90
 O      -0.065670     2.689859     0.651727     185.63
 C      -0.298239     0.303160     0.378574      25.58
 H       0.878532     0.333953     0.815516      17.69
 C      -2.556405    -0.484879    -0.351074      24.62
 C      -3.506910    -1.757575    -0.581836      74.38
 H      -4.356929    -1.229698    -1.259772      21.73
 O      -2.657691    -2.584823    -1.263447     230.91
 H      -2.950037    -3.544749    -1.600195      17.99
 C      -4.228231    -2.189328     0.726574     119.25
 H      -3.420682    -2.671620     1.238889      22.18
 O      -4.924134    -1.346659     1.584149     380.67
 H      -4.487217    -1.109312     2.379834      31.03
 C      -5.123087    -3.285126     0.340851      85.27
 O      -4.454185    -4.318221    -0.450487     319.16
 H      -3.979838    -4.936004     0.147930      28.78
 H      -6.086813    -2.902189    -0.188080      26.21
 H      -5.685918    -3.915924     1.337140      25.34
55
name = lig-etoh-frame_395
 C       2.353703     1.881210    -2.038022      45.46
 H       1.585834     2.285111    -2.711560      18.76
 C       3.404204     1.342396     0.114548      65.18
 H       3.624735     1.433844     1.129171      20.18
 C       3.875963     0.184161    -0.427158      20.31
 O       4.647548    -0.844297     0.289095     237.79
 C       5.500049    -0.315883     1.235889     118.19
 H       5.090464    -0.110402     2.256009      26.33
 H       5.922357     0.664822     0.818034      26.24
 H       6.226570    -1.072392     1.515334      26.79
 C       3.646710    -0.113612    -1.797768      24.85
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 O       3.940575    -1.286559    -2.497050     234.02
 H       4.625746    -1.674983    -2.132193      28.18
 C       2.774317     0.633042    -2.418931      67.76
 H       2.330537     0.011939    -3.179524      24.22
 C       2.631430     2.273126    -0.679615      52.22
 C       2.045218     3.714620    -0.147519      99.49
 H       2.370638     4.396625    -0.929458      24.99
 O       2.676912     4.077624     1.068128     292.24
 H       3.662016     4.375201     1.059454      26.90
 C       0.527316     3.731918    -0.239555      66.82
 H       0.396734     3.403355    -1.299430      19.91
 C       0.117878     5.239293     0.142024     101.32
 O       0.476734     6.069493    -0.850630     255.86
 H      -0.069567     5.638366    -1.773382      22.52
 H       0.497893     5.509905     1.228524      23.20
 H      -0.954351     5.555425     0.382286      22.67
 C      -1.253755    -0.686420     0.189163      48.15
 H      -1.280772    -1.860416     0.705768      16.31
 C      -3.026476     0.815213    -0.495385      48.18
 H      -4.101192     0.864412    -0.867520      24.20
 C      -2.315962     1.926711     0.071848       0.80
 O      -2.780092     3.135516     0.568122     215.58
 C      -4.084556     3.213889     1.239456     119.75
 H      -4.921725     3.146497     0.551196      26.77
 H      -4.284510     2.328416     1.775956      26.66
 H      -4.292753     4.233303     1.694835      25.32
 C      -0.874667     1.645213     0.221962       5.15
 O      -0.007703     2.660365     0.608343     191.73
 C      -0.317778     0.347072     0.393850      41.88
 H       0.590495     0.524617     0.821094      19.93
 C      -2.506690    -0.482329    -0.308663      31.94
 C      -3.514510    -1.664588    -0.572920      79.69
 H      -4.249836    -1.450899    -1.284523      22.56
 O      -2.653416    -2.612967    -1.244852     281.51
 H      -3.060107    -3.332298    -1.621750      25.12
 C      -4.201310    -2.243850     0.733776      96.98
 H      -3.413853    -2.592016     1.507163      18.57
 O      -4.924643    -1.330141     1.590382     285.13
 H      -4.299783    -1.532836     2.581038      18.73
 C      -5.175505    -3.321884     0.352110     109.97
 O      -4.458875    -4.241376    -0.407306     375.73
 H      -4.003002    -4.912522     0.095355      28.92
 H      -5.814205    -3.021722    -0.469636      27.55
 H      -5.384767    -3.794315     1.168532      29.86
55
name = lig-etoh-frame_396
 C       2.369219     1.867505    -1.930307      52.07
 H       1.467094     2.213966    -2.460718      18.65
 C       3.397258     1.309380     0.175455      60.52
 H       3.654767     1.531923     1.252380      19.81
 C       3.880701     0.149971    -0.408937      18.41
 O       4.625070    -0.891077     0.260576     226.16
 C       5.589509    -0.302190     1.259984     102.59
 H       4.992977    -0.063055     2.170397      25.73
 H       5.997056     0.510537     0.697596      27.35
 H       6.296600    -1.164313     1.464836      25.90
 C       3.696305    -0.157198    -1.816952      10.87
 O       3.949627    -1.329361    -2.504269     159.40
 H       4.702105    -1.907631    -1.913848      20.12
 C       2.802079     0.660970    -2.451998      62.89
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 H       2.413937     0.061119    -3.408272      22.02
 C       2.520931     2.326466    -0.631248      57.44
 C       2.035680     3.702025    -0.143145      81.87
 H       2.335640     4.705310    -0.923684      20.72
 O       2.670191     4.075022     1.111441     282.25
 H       3.547806     4.201223     0.762624      30.16
 C       0.462618     3.716105    -0.219025      91.42
 H       0.449649     3.708117    -1.348689      19.68
 C       0.055665     5.154129     0.180497     114.67
 O       0.433855     6.050948    -0.878899     318.80
 H       0.143723     5.652460    -1.626303      34.25
 H       0.500500     5.535941     1.052508      25.73
 H      -1.006557     5.142426     0.405712      25.43
 C      -1.225842    -0.743735     0.249267      53.19
 H      -0.890741    -1.643326     0.474567      21.01
 C      -3.039583     0.784954    -0.558487      59.64
 H      -4.037461     0.761823    -0.891707      25.10
 C      -2.319002     1.867030     0.058673      -1.87
 O      -2.733888     3.130192     0.577783     187.77
 C      -4.036847     3.310378     1.155864     102.79
 H      -4.903321     3.354142     0.348752      23.99
 H      -4.023193     2.395373     2.071662      21.20
 H      -4.271376     4.146469     1.777225      25.68
 C      -0.920834     1.660760     0.170391      20.17
 O       0.054824     2.650088     0.591534     185.50
 C      -0.407077     0.415417     0.392093      26.53
 H       0.679667     0.376265     0.917755      17.99
 C      -2.521657    -0.471595    -0.291726      27.35
 C      -3.486999    -1.557527    -0.551145      64.75
 H      -4.347879    -1.400358    -1.340843      20.67
 O      -2.616973    -2.645845    -1.238486     183.34
 H      -3.457335    -3.274770    -1.469649      17.56
 C      -4.146021    -2.284551     0.765771      88.69
 H      -3.376218    -2.739272     1.339275      21.82
 O      -4.906823    -1.303297     1.631383     337.97
 H      -4.543747    -1.463255     2.411195      29.46
 C      -5.195149    -3.352300     0.334850      69.66
 O      -4.451026    -4.230775    -0.417967     321.33
 H      -3.879324    -4.824547     0.260196      23.73
 H      -5.945927    -2.934426    -0.412623      26.54
 H      -5.661107    -3.807552     1.472911      26.39
55
name = lig-etoh-frame_397
 C       2.306026     1.862277    -1.846540      23.56
 H       1.491360     2.402550    -2.345137      17.75
 C       3.350102     1.351097     0.221191      53.03
 H       3.681135     1.676213     1.236625      20.28
 C       3.916646     0.067813    -0.414126      23.95
 O       4.601050    -0.918180     0.238844     215.01
 C       5.651567    -0.324001     1.266466      87.57
 H       5.018488     0.098916     2.079179      24.96
 H       6.273759     0.513046     0.770917      26.36
 H       6.389133    -1.154243     1.425835      25.43
 C       3.728493    -0.210832    -1.796648      20.60
 O       3.997758    -1.389052    -2.483112     186.87
 H       4.530638    -2.074567    -1.888104      20.27
 C       2.819230     0.672977    -2.536235      50.76
 H       2.471510     0.537789    -3.520586      25.12
 C       2.503510     2.317475    -0.547642      36.48
 C       2.041028     3.694876    -0.164926      90.16
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 H       2.299513     4.542674    -0.853381      21.86
 O       2.651814     4.073166     1.149707     270.16
 H       3.659574     4.078219     0.705852      25.08
 C       0.473157     3.735769    -0.197171      78.84
 H       0.101989     3.742607    -1.278612      17.27
 C      -0.045029     5.062144     0.228585      90.64
 O       0.397254     6.055722    -0.886671     141.20
 H       0.236888     5.654265    -1.979673      22.83
 H       0.715189     5.525896     1.028019      21.48
 H      -1.145855     4.747374     0.315608      21.69
 C      -1.205617    -0.747337     0.293511      32.83
 H      -0.456321    -1.775959     0.330315      17.59
 C      -3.053063     0.795815    -0.564340      56.65
 H      -4.134843     0.890988    -0.885378      23.64
 C      -2.323998     1.844405     0.037531       2.86
 O      -2.678497     3.139180     0.562589     193.64
 C      -4.015630     3.339651     1.093719     118.98
 H      -4.729797     3.332282     0.329373      26.47
 H      -4.131470     2.661386     1.892332      26.02
 H      -3.887722     4.313380     1.725690      24.45
 C      -0.937603     1.725835     0.153006      18.51
 O       0.079209     2.631921     0.582926     188.49
 C      -0.476580     0.423533     0.408468      24.05
 H       0.527586     0.143407     0.738364      19.40
 C      -2.535719    -0.487078    -0.279658      25.15
 C      -3.454399    -1.533188    -0.539442      74.19
 H      -4.255368    -1.131950    -1.120680      22.57
 O      -2.613553    -2.677079    -1.244606     160.99
 H      -3.449830    -3.277248    -1.154932      16.10
 C      -4.133702    -2.270966     0.791453      78.89
 H      -3.255091    -2.907932     1.172734      20.18
 O      -4.885281    -1.281520     1.634622     276.12
 H      -4.530098    -1.254873     2.744326      21.23
 C      -5.218189    -3.346672     0.373621     106.48
 O      -4.436542    -4.302153    -0.439892     360.91
 H      -3.776632    -4.575058     0.200035      30.73
 H      -6.107293    -2.854406    -0.039105      28.06
 H      -5.841074    -3.655298     1.074828      29.79
55
name = lig-etoh-frame_398
 C       2.211497     1.830231    -1.823511      43.80
 H       1.671017     2.596897    -2.435473      21.36
 C       3.316092     1.386580     0.227546      43.30
 H       3.712158     1.701780     1.165078      23.69
 C       3.920131     0.051377    -0.419659      15.45
 O       4.617962    -0.932493     0.257296     217.05
 C       5.694454    -0.350372     1.226883     108.83
 H       5.225440     0.119552     2.092008      26.42
 H       6.314215     0.432968     0.881931      28.08
 H       6.327208    -1.174487     1.556976      26.59
 C       3.686359    -0.238684    -1.807661      21.18
 O       4.057604    -1.454560    -2.446694     227.82
 H       4.466858    -2.074552    -1.923912      26.17
 C       2.840690     0.721181    -2.552784      50.66
 H       2.606142     0.946160    -3.711419      19.44
 C       2.565975     2.230488    -0.461876      29.50
 C       2.031069     3.670859    -0.155645      81.39
 H       2.495146     4.418063    -1.097937      18.60
 O       2.644610     4.072207     1.145615     326.17
 H       3.594756     4.120371     1.219866      27.28
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 C       0.521136     3.752958    -0.198719      88.36
 H      -0.051951     3.475266    -1.117388      18.51
 C      -0.112426     5.010544     0.248823     105.42
 O       0.342381     6.047774    -0.904387     224.81
 H       0.147433     5.756073    -1.759069      30.98
 H       0.375276     5.371157     1.067678      26.04
 H      -1.160781     4.883468     0.383513      25.01
 C      -1.210030    -0.743029     0.297295      54.02
 H      -0.660819    -1.599213     0.189292      20.14
 C      -3.076489     0.818691    -0.508652      57.95
 H      -4.089123     1.057196    -0.785334      24.54
 C      -2.313780     1.904578     0.019654       1.73
 O      -2.631549     3.139219     0.519790     187.52
 C      -3.952728     3.397654     1.055029     106.34
 H      -4.801071     3.368032     0.188233      24.10
 H      -4.538931     2.550897     1.863267      21.86
 H      -3.692096     4.385262     1.306101      24.92
 C      -0.898754     1.753734     0.179135      19.30
 O       0.065256     2.608423     0.590386     192.10
 C      -0.510548     0.396704     0.418207      26.42
 H       0.600839     0.245914     0.608370      19.72
 C      -2.508123    -0.508097    -0.251686      26.11
 C      -3.431535    -1.601366    -0.523630      69.59
 H      -4.275798    -1.037779    -1.093646      20.82
 O      -2.651245    -2.683262    -1.239090     185.37
 H      -3.213315    -3.551702    -1.130644      14.34
 C      -4.149049    -2.238905     0.815275      93.22
 H      -3.297963    -2.748456     1.255965      21.82
 O      -4.843370    -1.279068     1.651175     362.14
 H      -4.348202    -0.991794     2.535390      25.21
 C      -5.215468    -3.287571     0.390653      75.71
 O      -4.456826    -4.383348    -0.458178     292.93
 H      -3.645473    -4.580358     0.161871      24.76
 H      -6.022937    -2.752527    -0.191048      26.13
 H      -5.888647    -3.964795     1.275352      25.50
55
name = lig-etoh-frame_399
 C       2.159662     1.782744    -1.832468      51.84
 H       1.897812     2.604948    -2.495887      23.61
 C       3.369965     1.318613     0.238611      40.21
 H       3.813381     1.649792     1.265365      21.69
 C       3.881239     0.097700    -0.434953       6.66
 O       4.671094    -0.923074     0.309241     228.00
 C       5.706132    -0.392482     1.185582     106.00
 H       5.308714     0.050757     2.172555      24.85
 H       6.358973     0.413187     0.669593      25.52
 H       6.212465    -1.325478     1.674820      24.48
 C       3.605876    -0.256105    -1.824782      -3.76
 O       4.099244    -1.478790    -2.423086     130.04
 H       4.677604    -2.144432    -1.662930      19.66
 C       2.840217     0.818831    -2.538814      54.56
 H       2.920647     0.848921    -3.559727      21.72
 C       2.564693     2.166500    -0.480249      37.03
 C       2.110076     3.628884    -0.150853      83.11
 H       2.548037     4.211606    -1.028955      20.53
 O       2.601597     4.084806     1.141335     323.31
 H       3.550472     4.188902     1.410166      26.15
 C       0.533688     3.723323    -0.206459      68.08
 H       0.221104     3.303939    -1.246165      17.73
 C      -0.145498     5.021489     0.209085      92.10
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 O       0.276210     6.041335    -0.857408     223.66
 H      -0.137203     5.597213    -1.825230      22.79
 H       0.096378     5.397181     1.345917      22.49
 H      -1.263191     5.109761     0.353268      22.85
 C      -1.275517    -0.715646     0.256693      52.75
 H      -0.848442    -1.863272     0.185118      15.51
 C      -3.066171     0.843183    -0.389066      58.59
 H      -4.118274     1.037166    -0.678206      24.41
 C      -2.250229     1.968784     0.001793      10.05
 O      -2.617504     3.144552     0.470887     217.19
 C      -3.941363     3.435192     0.981428     126.75
 H      -4.615302     3.521870     0.206634      27.70
 H      -4.370833     2.806439     1.681704      28.27
 H      -3.892125     4.574979     1.188923      25.10
 C      -0.867250     1.692677     0.226986      29.32
 O       0.053183     2.603738     0.641574     195.75
 C      -0.453052     0.409245     0.423108      35.95
 H       0.696847     0.495788     0.531350      19.10
 C      -2.509747    -0.504316    -0.228806      37.58
 C      -3.445550    -1.705230    -0.516662      75.87
 H      -4.243191    -1.372964    -1.187335      21.10
 O      -2.708176    -2.672654    -1.230962     244.26
 H      -2.953080    -3.691856    -1.214653      14.86
 C      -4.162322    -2.205355     0.836694      99.54
 H      -3.368928    -2.588813     1.546033      19.84
 O      -4.801725    -1.266344     1.647840     384.93
 H      -4.071453    -1.021330     2.349195      25.21
 C      -5.217496    -3.273599     0.412794      89.15
 O      -4.496591    -4.442780    -0.456063     295.59
 H      -3.771229    -4.815466     0.167473      24.38
 H      -5.753352    -2.862296    -0.450031      26.55
 H      -5.425769    -3.844770     1.166685      28.61
55
name = lig-etoh-frame_400
 C       2.160992     1.780082    -1.841525      56.17
 H       1.878544     2.614800    -2.499888      21.74
 C       3.466003     1.216629     0.249884      43.51
 H       3.815630     1.467269     1.172995      22.41
 C       3.848414     0.118156    -0.439397       6.37
 O       4.709088    -0.888345     0.344802     231.69
 C       5.711613    -0.437709     1.179261     128.17
 H       5.299970     0.061544     2.037078      27.36
 H       6.324561     0.167852     0.571844      27.71
 H       6.206252    -1.321878     1.470393      26.80
 C       3.528269    -0.258100    -1.803838       3.05
 O       4.130673    -1.474968    -2.376406     198.73
 H       4.719423    -1.758768    -1.713143      23.62
 C       2.875432     0.824223    -2.507077      52.50
 H       3.090402     0.647750    -3.651451      18.97
 C       2.517968     2.121300    -0.541457      23.91
 C       2.209840     3.557658    -0.116202      75.14
 H       2.659524     4.300634    -1.050152      20.08
 O       2.529997     4.105479     1.148008     255.10
 H       3.621887     4.226250     1.131174      23.33
 C       0.530556     3.647807    -0.216418      66.23
 H       0.506472     3.482382    -1.307477      18.41
 C      -0.169449     5.089720     0.169884     109.75
 O       0.196668     6.021072    -0.801054     330.68
 H      -0.230165     5.613453    -1.638068      27.15
 H       0.089133     5.349035     1.123386      25.64
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 H      -1.254957     5.001333     0.053201      23.07
 C      -1.275690    -0.720256     0.200701      44.51
 H      -1.159625    -1.807041     0.398481      18.29
 C      -3.039383     0.868881    -0.246776      71.58
 H      -4.114097     0.918945    -0.502807      17.26
 C      -2.183355     1.952312    -0.011985      20.49
 O      -2.622797     3.201690     0.431270     209.54
 C      -3.929303     3.526978     0.855559      86.82
 H      -4.680763     3.505628    -0.095851      23.27
 H      -4.150953     2.799688     1.927913      21.99
 H      -4.099072     4.474527     1.356957      25.69
 C      -0.857891     1.636368     0.280252      28.27
 O       0.055970     2.630706     0.721880     194.34
 C      -0.338940     0.393893     0.411991      39.25
 H       0.689626     0.375220     0.615547      19.52
 C      -2.604085    -0.477475    -0.235156      37.02
 C      -3.479625    -1.779793    -0.496258      74.98
 H      -4.331628    -1.598195    -1.263774      19.44
 O      -2.718354    -2.682202    -1.243015     285.08
 H      -3.098244    -3.513013    -1.093782      18.23
 C      -4.143570    -2.218102     0.835180      94.94
 H      -3.447531    -2.698887     1.559408      20.07
 O      -4.784365    -1.217121     1.640284     353.05
 H      -3.840464    -1.096554     2.299332      19.59
 C      -5.127383    -3.288741     0.371406      76.48
 O      -4.542410    -4.491131    -0.435759     297.60
 H      -4.030118    -5.005667     0.204660      27.63
 H      -5.861403    -3.009953    -0.433528      26.13
 H      -5.530133    -3.816198     1.464313      25.45
55
name = lig-etoh-frame_401
 C       2.200079     1.828610    -1.873764      38.04
 H       1.641396     2.584769    -2.449193      19.30
 C       3.480020     1.194494     0.195502      33.22
 H       3.879072     1.378442     1.289005      19.87
 C       3.868307     0.041892    -0.415976      22.35
 O       4.683399    -0.864402     0.316689     248.00
 C       5.725416    -0.467192     1.180130     109.15
 H       5.362658     0.201433     2.046915      25.06
 H       6.499443     0.153599     0.592104      26.05
 H       6.374938    -1.439154     1.376746      24.23
 C       3.490321    -0.262523    -1.755203      22.92
 O       4.125272    -1.407336    -2.328101     189.07
 H       4.900007    -1.589292    -1.637823      21.01
 C       2.945424     0.708367    -2.523805      53.72
 H       2.894570     0.642962    -3.583355      19.20
 C       2.531919     2.063426    -0.530390      34.50
 C       2.227348     3.511662    -0.100155      88.04
 H       2.692597     4.294484    -0.894939      20.43
 O       2.509313     4.123488     1.147193     313.01
 H       3.383346     4.266580     0.998278      29.76
 C       0.559895     3.604821    -0.198202      53.79
 H       0.391933     3.558630    -1.361802      16.67
 C      -0.186917     5.086712     0.109264      99.08
 O       0.135283     6.039591    -0.758403     325.90
 H      -0.152813     5.748432    -1.704869      27.29
 H       0.235636     5.447884     1.168094      22.33
 H      -1.225818     4.754745     0.105216      21.52
 C      -1.264163    -0.708760     0.149597      34.92
 H      -1.076653    -1.789021     0.531617      17.57
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 C      -3.054042     0.868219    -0.133710      74.89
 H      -4.108117     1.041896    -0.258602      17.48
 C      -2.165533     1.923060     0.016211      16.01
 O      -2.605379     3.291098     0.381836     222.38
 C      -3.959785     3.565450     0.753195     118.01
 H      -4.649177     3.354423     0.024638      27.01
 H      -4.126540     2.894182     1.557060      26.65
 H      -3.997579     4.514349     1.342847      25.82
 C      -0.807984     1.644332     0.343399      15.04
 O       0.054743     2.668597     0.789540     200.62
 C      -0.274543     0.293769     0.379385      36.48
 H       0.820728     0.012912     0.846037      16.59
 C      -2.676821    -0.461448    -0.238901      15.29
 C      -3.525385    -1.750393    -0.492234      81.62
 H      -4.435556    -1.519846    -1.071886      22.68
 O      -2.692298    -2.715311    -1.255299     218.04
 H      -3.353970    -3.542741    -0.995786      13.19
 C      -4.114504    -2.283891     0.808731      96.68
 H      -3.390907    -2.918047     1.331409      22.82
 O      -4.743773    -1.159761     1.626824     354.91
 H      -4.236366    -1.015757     2.366004      31.52
 C      -5.070446    -3.385077     0.367895     119.54
 O      -4.594562    -4.515565    -0.403330     296.93
 H      -4.178074    -5.190857     0.306605      27.29
 H      -6.004604    -3.012682    -0.100782      28.52
 H      -5.707475    -3.521451     1.142993      29.13
55
name = lig-etoh-frame_402
 C       2.298478     1.831491    -1.921189      54.40
 H       1.501193     2.415304    -2.400270      18.57
 C       3.451299     1.222584     0.149216      45.86
 H       3.792156     1.418285     1.103020      20.28
 C       3.896154    -0.041119    -0.364622      34.19
 O       4.641192    -0.877281     0.260886     253.30
 C       5.781872    -0.475136     1.172979     120.52
 H       5.532928     0.063830     2.052061      27.85
 H       6.448316     0.231299     0.733790      28.34
 H       6.234820    -1.341887     1.482584      27.51
 C       3.528414    -0.311158    -1.696949      31.47
 O       4.109653    -1.323416    -2.271083     166.00
 H       5.044438    -1.625195    -1.746108      21.09
 C       2.926078     0.647357    -2.547070      50.95
 H       2.688391     0.534463    -3.639695      20.48
 C       2.595160     2.033759    -0.491696      44.66
 C       2.134107     3.484820    -0.103559      92.48
 H       2.712033     4.219394    -0.871838      23.17
 O       2.508681     4.127850     1.149680     240.54
 H       3.550005     4.438445     1.155000      25.59
 C       0.611294     3.631662    -0.188662      72.72
 H       0.112087     3.284196    -1.106901      22.19
 C      -0.165802     4.986321     0.123192     102.93
 O       0.086513     6.113304    -0.765799     272.75
 H       0.083757     5.907522    -1.857117      25.22
 H       0.174906     5.435911     1.028851      24.27
 H      -1.196208     4.666901     0.373551      21.93
 C      -1.274128    -0.711110     0.099199      34.56
 H      -0.830057    -1.743434     0.447971      15.16
 C      -3.118294     0.861547    -0.058923      53.57
 H      -4.170990     1.273988    -0.014955      16.90
 C      -2.151983     1.932883     0.105879      -2.49
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 O      -2.562167     3.360618     0.309450     185.15
 C      -3.970876     3.580601     0.688678      91.43
 H      -4.846136     3.362852    -0.130119      23.51
 H      -4.373563     2.630801     1.465383      21.33
 H      -3.888455     4.648088     1.010526      24.06
 C      -0.717503     1.650501     0.405457      -9.18
 O       0.047292     2.700613     0.838841     198.99
 C      -0.258788     0.195224     0.359813      41.67
 H       0.551898    -0.143083     0.825712      19.32
 C      -2.661138    -0.478160    -0.221212      25.63
 C      -3.546158    -1.648458    -0.499801      70.95
 H      -4.493294    -1.296808    -1.022112      22.81
 O      -2.699636    -2.760423    -1.239843     201.96
 H      -3.224642    -3.604217    -1.229936      18.83
 C      -4.076416    -2.356831     0.790086      77.36
 H      -3.186056    -2.872900     1.269295      22.71
 O      -4.710972    -1.138298     1.564066     223.38
 H      -4.463118    -1.066228     2.691615      22.55
 C      -5.112545    -3.457831     0.375239      91.40
 O      -4.655067    -4.542004    -0.357895     332.27
 H      -4.171871    -5.132987     0.215841      31.66
 H      -5.887960    -2.847220    -0.183576      28.57
 H      -5.827980    -3.738495     1.375887      27.20
55
name = lig-etoh-frame_403
 C       2.422158     1.768132    -1.943266      66.48
 H       1.572190     2.258865    -2.439931      19.22
 C       3.448632     1.209694     0.143766      53.09
 H       3.766759     1.614952     1.179715      16.12
 C       3.850630    -0.009066    -0.341170      27.81
 O       4.666888    -0.950921     0.257782     256.21
 C       5.809567    -0.465004     1.157627      91.10
 H       5.408948    -0.067043     2.189266      24.67
 H       6.410066     0.326976     0.646323      26.50
 H       6.219023    -1.510561     1.560230      23.93
 C       3.583177    -0.305994    -1.645391      29.70
 O       4.137984    -1.317211    -2.256154     225.23
 H       4.836620    -1.677495    -1.901739      27.21
 C       2.833819     0.649878    -2.545175      67.96
 H       2.594032     0.241771    -3.573810      22.50
 C       2.622342     2.080674    -0.534384      78.53
 C       2.060284     3.481808    -0.110632      92.81
 H       2.558261     4.138191    -1.036653      24.39
 O       2.529412     4.126489     1.158571     281.53
 H       3.502218     4.402945     1.262749      27.80
 C       0.612168     3.670569    -0.187800      74.71
 H       0.063105     2.994826    -0.934183      21.86
 C      -0.107736     4.894187     0.149756      97.97
 O       0.048429     6.193986    -0.801877     267.97
 H       0.056265     5.838352    -1.631359      31.50
 H       0.271726     5.354645     1.139402      24.25
 H      -1.156276     4.741381     0.344606      23.02
 C      -1.276489    -0.750091     0.050602      44.34
 H      -0.912757    -1.780020     0.106369      16.00
 C      -3.155491     0.893742     0.000996      41.26
 H      -4.175592     1.175893     0.075939      18.65
 C      -2.120380     1.940865     0.229311     -15.81
 O      -2.534025     3.370087     0.237734     180.15
 C      -4.002938     3.545179     0.616556     128.31
 H      -4.601281     3.617304    -0.235965      27.24
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 H      -4.348125     2.920406     1.377979      28.70
 H      -4.038799     4.610647     0.807527      26.30
 C      -0.663693     1.618788     0.450068       4.03
 O       0.052295     2.722009     0.902879     178.72
 C      -0.318852     0.209640     0.344616      47.40
 H       0.692568    -0.259398     0.861242      16.07
 C      -2.609785    -0.478693    -0.186033      23.94
 C      -3.560351    -1.590397    -0.505493      60.74
 H      -4.386434    -1.162137    -1.146281      21.76
 O      -2.722537    -2.772699    -1.225635     224.32
 H      -3.196498    -3.588815    -1.362790      20.11
 C      -4.037474    -2.389958     0.785057      83.05
 H      -3.157310    -2.588738     1.330401      23.98
 O      -4.681475    -1.152259     1.505472     298.98
 H      -4.508152    -1.407764     2.412503      28.30
 C      -5.232812    -3.468601     0.449601      94.58
 O      -4.726535    -4.581104    -0.338070     323.25
 H      -3.970710    -5.031931     0.223461      24.66
 H      -5.691887    -2.905678    -0.374462      27.47
 H      -5.515374    -3.971977     1.287003      28.01
55
name = lig-etoh-frame_404
 C       2.470915     1.750457    -1.937195      51.84
 H       1.797315     2.341069    -2.573619      19.13
 C       3.443616     1.248381     0.221163      64.83
 H       3.747372     1.644536     1.182277      15.55
 C       3.819794     0.032173    -0.316806       6.23
 O       4.729132    -1.031210     0.293129     243.73
 C       5.782595    -0.488328     1.176216     103.40
 H       5.280230    -0.126945     2.013317      28.09
 H       6.340005     0.286652     0.611831      28.18
 H       6.371653    -1.340908     1.307351      27.50
 C       3.601371    -0.230699    -1.664625      11.90
 O       4.164638    -1.362498    -2.301689     149.61
 H       4.937622    -1.964856    -1.711526      17.87
 C       2.784287     0.549883    -2.504967      56.33
 H       2.527276     0.151785    -3.430753      24.76
 C       2.640035     2.147689    -0.623019      96.03
 C       2.087374     3.515576    -0.132304      85.85
 H       2.241260     4.144221    -1.112788      24.81
 O       2.537385     4.110005     1.156856     311.05
 H       3.491609     4.216904     1.065641      28.65
 C       0.549513     3.614365    -0.186223      71.58
 H       0.335680     3.185619    -1.155976      19.93
 C      -0.046252     4.930560     0.184379      96.87
 O       0.020848     6.237602    -0.802878     206.02
 H      -0.114771     5.630850    -1.744942      24.11
 H       0.451364     5.159564     1.168479      23.73
 H      -1.129267     4.786154     0.133789      20.63
 C      -1.263674    -0.794849     0.007092      39.75
 H      -1.086350    -1.940237    -0.423995      14.52
 C      -3.090510     0.926101     0.059363      47.36
 H      -4.226680     0.959664     0.040345      19.46
 C      -2.114948     1.929863     0.340422      -9.44
 O      -2.528283     3.321342     0.192680     169.16
 C      -3.986773     3.555309     0.498776      94.92
 H      -4.480065     3.539747    -0.565287      23.53
 H      -4.401240     3.043908     1.617375      24.02
 H      -4.147532     4.639137     0.908990      24.63
 C      -0.691229     1.591990     0.490536      19.40
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 O       0.071066     2.719680     0.993195     163.90
 C      -0.340151     0.265647     0.376206      50.50
 H       0.611896    -0.007151     0.567300      19.47
 C      -2.600265    -0.430796    -0.144334      38.91
 C      -3.551866    -1.622137    -0.516447      71.35
 H      -4.292651    -1.249699    -1.240775      20.45
 O      -2.738103    -2.739469    -1.220209     193.93
 H      -3.504540    -3.525112    -1.368930      14.47
 C      -4.054504    -2.336382     0.758516      92.88
 H      -3.143577    -2.541610     1.437656      20.28
 O      -4.662452    -1.211732     1.436736     346.97
 H      -4.456097    -1.511469     2.357509      27.76
 C      -5.259256    -3.451090     0.497033      76.93
 O      -4.780805    -4.645805    -0.327177     301.13
 H      -3.864299    -4.775438     0.127616      24.27
 H      -5.997541    -2.999512    -0.248533      26.03
 H      -5.657095    -3.980407     1.496442      25.59
55
name = lig-etoh-frame_405
 C       2.437683     1.785883    -1.960464      36.20
 H       2.047252     2.536845    -2.650497      18.33
 C       3.407578     1.331279     0.289692      48.63
 H       3.759374     1.603531     1.290716      17.19
 C       3.855443     0.032572    -0.270099      -8.53
 O       4.763797    -1.075228     0.315382     226.75
 C       5.733440    -0.517071     1.158347      97.71
 H       5.243065    -0.068088     2.128960      24.83
 H       6.280132     0.309930     0.677462      27.80
 H       6.655899    -1.262225     1.248332      24.83
 C       3.642649    -0.235475    -1.719933      14.15
 O       4.204000    -1.419465    -2.343706     189.75
 H       4.625538    -1.931716    -1.584516      19.72
 C       2.768278     0.419986    -2.437821      47.28
 H       2.417676     0.158185    -3.531314      22.34
 C       2.702056     2.198663    -0.650910      43.42
 C       2.104652     3.560284    -0.165174      78.71
 H       2.279165     4.453587    -1.121477      20.90
 O       2.550747     4.080054     1.115632     244.58
 H       3.626775     4.030941     0.870240      23.66
 C       0.519410     3.511178    -0.168753      63.90
 H       0.377002     3.432533    -1.316800      16.47
 C      -0.009536     5.034392     0.193662      96.57
 O       0.015031     6.207493    -0.804976     256.94
 H      -0.296307     5.879299    -1.669755      29.10
 H       0.454682     5.231482     1.153508      24.84
 H      -1.087749     4.839562     0.209571      21.62
 C      -1.246870    -0.815328    -0.059028      35.46
 H      -1.028047    -1.674934    -0.523832      19.13
 C      -3.002191     0.908613     0.116588      61.42
 H      -4.062682     0.989230    -0.021675      21.87
 C      -2.147887     1.925919     0.414192      12.53
 O      -2.536346     3.245504     0.191020     224.77
 C      -3.960814     3.598966     0.401550     127.85
 H      -4.496885     3.237650    -0.449839      27.39
 H      -4.340623     3.020240     1.165360      30.25
 H      -4.000160     4.574968     0.756592      26.84
 C      -0.787840     1.623855     0.558046      22.81
 O       0.088630     2.689924     1.048869     160.03
 C      -0.350384     0.283534     0.396853      26.42
 H       0.862253     0.201694     0.331173      17.59
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 C      -2.608590    -0.398053    -0.107580      27.10
 C      -3.500615    -1.683932    -0.540269      69.91
 H      -4.358393    -1.408671    -1.273696      19.45
 O      -2.780413    -2.701861    -1.227107     284.08
 H      -3.513885    -3.236070    -1.304611      21.86
 C      -4.108646    -2.261399     0.721724     107.66
 H      -3.330644    -2.802154     1.232185      22.34
 O      -4.670927    -1.280236     1.392187     323.43
 H      -4.411198    -1.227309     2.508364      23.35
 C      -5.246742    -3.455109     0.530591      90.50
 O      -4.815829    -4.684591    -0.304972     339.13
 H      -3.935452    -4.817228     0.023299      31.07
 H      -6.267923    -3.078745     0.207180      27.21
 H      -5.762806    -3.587029     1.451185      27.02
55
name = lig-etoh-frame_406
 C       2.406113     1.782329    -1.988735      32.47
 H       2.021632     2.601668    -2.606441      20.24
 C       3.391721     1.354955     0.300844      35.50
 H       3.729757     1.619371     1.369033      18.97
 C       3.918776     0.031766    -0.249727      -1.32
 O       4.747577    -1.078024     0.311165     258.60
 C       5.731647    -0.523465     1.162821     120.76
 H       5.451933    -0.258725     2.149639      28.56
 H       6.099547     0.459667     0.733638      27.71
 H       6.558623    -1.146873     1.405073      27.35
 C       3.734396    -0.355393    -1.707060      -3.94
 O       4.223976    -1.450182    -2.357832     218.95
 H       4.514895    -1.955790    -1.586708      21.42
 C       2.692207     0.419267    -2.425916      46.00
 H       2.482346     0.160503    -3.396528      24.54
 C       2.777998     2.252069    -0.636780      26.52
 C       2.091661     3.614911    -0.234869     113.38
 H       2.391471     4.503155    -0.742570      22.41
 O       2.605529     4.034812     1.035085     314.88
 H       3.533511     4.065961     1.088252      30.73
 C       0.552580     3.495310    -0.140762      66.21
 H       0.018546     3.258387    -1.069036      21.73
 C      -0.015748     5.111401     0.164404      91.31
 O       0.037247     6.157110    -0.784680     267.96
 H      -0.389124     5.952863    -1.668997      27.03
 H       0.458393     5.614195     1.149508      22.83
 H      -1.042336     4.919466     0.562028      23.46
 C      -1.219486    -0.715125    -0.089538      36.50
 H      -0.675351    -1.750600    -0.563612      16.51
 C      -2.976961     0.844879     0.161065      47.91
 H      -4.002635     1.214999    -0.055201      19.91
 C      -2.186268     1.945492     0.458819      24.61
 O      -2.548807     3.186664     0.215224     237.26
 C      -3.906843     3.605634     0.301727     103.78
 H      -4.634513     3.214711    -0.522846      24.70
 H      -4.431452     2.725887     1.088293      23.16
 H      -3.883087     4.773175     0.429102      23.88
 C      -0.861361     1.653880     0.666995       6.96
 O       0.094218     2.643597     1.037624     178.56
 C      -0.328889     0.275933     0.383218      26.69
 H       0.703244     0.332919     0.187413      20.43
 C      -2.587517    -0.465053    -0.101974      29.29
 C      -3.476044    -1.677383    -0.568496      85.90
 H      -4.344697    -1.382317    -1.165699      20.56
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 O      -2.803819    -2.666781    -1.246831     253.94
 H      -3.544818    -3.399911    -1.420113      16.44
 C      -4.166643    -2.292796     0.660168      93.97
 H      -3.418400    -2.992144     1.091520      18.44
 O      -4.724523    -1.279747     1.428021     406.75
 H      -4.313427    -1.078168     2.177920      33.15
 C      -5.245766    -3.444778     0.532593      76.84
 O      -4.867401    -4.678318    -0.263506     292.24
 H      -3.934085    -5.070570     0.089862      25.47
 H      -6.254634    -3.108078     0.211650      26.92
 H      -5.461935    -3.566546     1.743438      26.29
55
name = lig-etoh-frame_407
 C       2.406210     1.754403    -1.968299      40.58
 H       1.773394     2.428667    -2.572789      19.85
 C       3.420871     1.316099     0.264953      21.77
 H       3.640470     1.643776     1.217427      20.77
 C       3.977475     0.016666    -0.298137      10.49
 O       4.701802    -1.043752     0.310073     262.03
 C       5.762247    -0.488192     1.192592      97.48
 H       5.366998    -0.412390     2.300981      25.02
 H       5.996102     0.479042     0.796229      26.53
 H       6.580712    -1.300914     1.357942      24.39
 C       3.740911    -0.410924    -1.652484       1.35
 O       4.237940    -1.470273    -2.350445     177.91
 H       4.697406    -2.293341    -1.670536      18.82
 C       2.666713     0.475462    -2.390899      51.78
 H       2.469392     0.080519    -3.479558      23.09
 C       2.822850     2.281199    -0.653344      43.49
 C       2.111924     3.618402    -0.272239      95.79
 H       2.432346     4.636672    -1.037166      19.63
 O       2.641735     3.993619     0.993200     272.65
 H       3.665657     4.107863     1.113372      26.56
 C       0.560827     3.563671    -0.090938      52.67
 H      -0.154617     2.995171    -0.768306      19.61
 C      -0.038658     5.154157     0.196693     100.14
 O       0.076050     6.115838    -0.776565     225.45
 H      -0.433104     5.799272    -1.718974      23.15
 H       0.544065     5.700862     0.887896      24.15
 H      -0.986507     5.010450     0.730763      24.57
 C      -1.131720    -0.634431    -0.115023      58.40
 H      -0.702593    -1.483207    -0.273173      21.17
 C      -3.031891     0.779979     0.186037      45.15
 H      -4.028017     1.172277    -0.103675      17.34
 C      -2.202626     1.903603     0.490329       3.96
 O      -2.564863     3.187770     0.237575     247.00
 C      -3.906192     3.547323     0.219147     138.86
 H      -4.441001     3.492376    -0.735526      26.68
 H      -4.373611     3.147966     1.078265      29.20
 H      -3.933334     4.576679     0.218545      27.99
 C      -0.847268     1.630723     0.782737       8.55
 O       0.104361     2.608130     0.995622     173.38
 C      -0.346037     0.344661     0.361521      35.74
 H       0.780323     0.264865     0.170125      17.66
 C      -2.559749    -0.573939    -0.123060      24.57
 C      -3.514029    -1.624233    -0.571158      70.60
 H      -4.336769    -1.055626    -1.187489      19.67
 O      -2.807642    -2.667618    -1.300083     263.77
 H      -3.321263    -3.543470    -1.509164      18.95
 C      -4.204440    -2.378536     0.601695      85.44
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 H      -3.351887    -2.829277     1.170570      18.68
 O      -4.814504    -1.259770     1.464478     292.27
 H      -3.960070    -1.018575     2.201539      17.82
 C      -5.258774    -3.440607     0.566095     102.20
 O      -4.912606    -4.649267    -0.209293     335.15
 H      -4.229158    -5.131147     0.271694      29.41
 H      -6.153700    -3.158545    -0.001074      27.17
 H      -5.039077    -3.793096     1.523795      29.18
55
name = lig-etoh-frame_408
 C       2.404978     1.749246    -1.920117      73.80
 H       1.565675     2.154170    -2.530394      19.43
 C       3.474076     1.261159     0.155444      52.80
 H       3.653062     1.639526     1.264068      22.33
 C       4.012436     0.001052    -0.372436      32.47
 O       4.667234    -0.983708     0.337911     260.64
 C       5.776456    -0.484039     1.267706      98.69
 H       5.273587    -0.464828     2.192676      25.59
 H       6.137357     0.530110     0.915615      27.04
 H       6.531355    -1.255632     1.028764      23.61
 C       3.649943    -0.377602    -1.618767       9.80
 O       4.255727    -1.512311    -2.321519     268.07
 H       4.786314    -2.150497    -2.025571      29.67
 C       2.735291     0.466689    -2.365811      57.86
 H       2.373077     0.153001    -3.317451      23.09
 C       2.828346     2.253506    -0.700801      83.26
 C       2.183875     3.626035    -0.308721      87.17
 H       2.181364     4.134633    -1.227239      25.82
 O       2.673661     3.973613     0.995314     278.73
 H       3.704575     4.078712     0.754045      23.57
 C       0.506416     3.652565    -0.043211      45.81
 H       0.089842     3.148255    -0.961719      20.03
 C      -0.036603     5.139598     0.285983      96.33
 O       0.096448     6.082911    -0.831495     278.38
 H      -0.180428     5.678918    -1.589810      31.38
 H       0.874092     5.529436     0.987382      22.47
 H      -1.076324     5.097295     0.686993      23.95
 C      -1.102681    -0.604254    -0.125243      38.63
 H      -0.541393    -1.723793    -0.212923      16.47
 C      -3.100691     0.715505     0.183946      39.13
 H      -4.139128     0.842718    -0.104399      16.76
 C      -2.209354     1.798238     0.513304     -15.75
 O      -2.557609     3.204833     0.263546     180.85
 C      -3.938056     3.503154     0.123464     116.34
 H      -4.284416     3.362240    -0.923754      24.73
 H      -4.608241     3.576461     1.199769      23.20
 H      -3.912446     4.705601     0.225023      24.44
 C      -0.799691     1.602328     0.849834      18.09
 O       0.140721     2.602404     0.996654     171.23
 C      -0.321251     0.476443     0.349711      50.11
 H       0.770502     0.158870     0.381213      15.73
 C      -2.519164    -0.600092    -0.130119      14.48
 C      -3.594445    -1.600564    -0.589873      73.66
 H      -4.213972    -0.971442    -1.203564      20.58
 O      -2.787802    -2.674231    -1.379551     277.08
 H      -3.278827    -3.440410    -1.404472      23.60
 C      -4.207853    -2.384056     0.590898      93.44
 H      -3.346119    -2.602039     1.203824      20.35
 O      -4.881268    -1.254402     1.511167     305.75
 H      -4.013755    -1.136777     2.039773      19.84
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 C      -5.246724    -3.469358     0.563933      90.22
 O      -4.956218    -4.628439    -0.177122     342.20
 H      -4.377746    -5.124105     0.445119      28.35
 H      -6.251434    -3.104801     0.148229      26.23
 H      -5.262556    -3.957693     1.636943      25.54
55
name = lig-etoh-frame_409
 C       2.374747     1.714983    -1.912811      76.81
 H       1.541065     2.111490    -2.451172      19.97
 C       3.545944     1.241787     0.051194      43.58
 H       3.753199     1.433742     1.029380      22.63
 C       4.021313     0.024875    -0.389475      51.08
 O       4.656780    -0.910175     0.384693     252.73
 C       5.761869    -0.485676     1.291083     115.56
 H       5.347302    -0.505172     2.365653      24.75
 H       6.224640     0.482826     1.137636      29.37
 H       6.550214    -1.183126     1.049636      24.55
 C       3.572862    -0.384128    -1.668647      38.58
 O       4.223588    -1.505675    -2.315644     188.63
 H       5.099635    -2.111606    -1.922258      24.84
 C       2.826747     0.438423    -2.348935      57.58
 H       2.300606     0.135021    -3.278350      19.47
 C       2.806221     2.194043    -0.717135      39.48
 C       2.189401     3.554474    -0.294790      67.91
 H       2.209817     4.181891    -1.418927      20.82
 O       2.738853     3.986361     0.970684     297.55
 H       3.658155     4.060121     0.786226      26.28
 C       0.457916     3.697945    -0.035915      46.13
 H       0.248799     3.566993    -1.160427      14.53
 C       0.028352     5.107576     0.379403     106.14
 O       0.120552     6.052676    -0.864707     206.45
 H       0.009652     5.421256    -1.826620      21.21
 H       0.685049     5.301649     1.134411      25.69
 H      -1.017732     5.178712     0.670443      23.91
 C      -1.087347    -0.656696    -0.113516      48.87
 H      -0.570025    -1.520148    -0.292723      18.16
 C      -3.122561     0.655229     0.168115      38.91
 H      -4.247680     0.625403     0.017604      15.70
 C      -2.238996     1.721187     0.526727     -11.12
 O      -2.542613     3.179507     0.314292     150.23
 C      -3.988004     3.564500     0.069595     121.07
 H      -4.377640     2.963701    -0.819659      25.25
 H      -4.691615     3.395476     0.803346      28.81
 H      -3.832619     4.582535    -0.030447      27.03
 C      -0.796504     1.650049     0.853459       2.92
 O       0.192246     2.642067     1.036758     146.51
 C      -0.250037     0.477889     0.329569      39.70
 H       0.774334     0.309477     0.564067      15.13
 C      -2.491763    -0.555616    -0.123679      11.81
 C      -3.609767    -1.631351    -0.622339      54.97
 H      -4.331230    -1.076308    -1.380991      19.09
 O      -2.777654    -2.654091    -1.457577     221.85
 H      -3.428817    -3.484709    -1.253471      16.48
 C      -4.219438    -2.301174     0.633337      99.98
 H      -3.289659    -2.643126     1.208772      19.02
 O      -4.931645    -1.280993     1.527203     318.33
 H      -4.256877    -1.078437     2.230185      25.02
 C      -5.265623    -3.507677     0.597117     105.41
 O      -4.988006    -4.636181    -0.177543     322.85
 H      -4.326733    -5.194087     0.442338      26.26
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 H      -6.232832    -3.024343     0.452635      27.39
 H      -5.721824    -3.639810     1.595170      26.94
55
name = lig-etoh-frame_410
 C       2.331079     1.640354    -1.943704      48.18
 H       1.575988     2.268913    -2.499761      22.14
 C       3.622576     1.270127    -0.017512      28.31
 H       3.959098     1.429797     1.091912      17.16
 C       4.006856     0.042933    -0.410281      51.09
 O       4.671031    -0.837157     0.442895     276.24
 C       5.728307    -0.488331     1.319435     122.93
 H       5.591417    -0.626086     2.406166      27.58
 H       6.130058     0.557421     1.241438      29.46
 H       6.620637    -1.249784     1.286358      24.78
 C       3.626166    -0.478196    -1.694086      32.33
 O       4.179385    -1.510448    -2.320194     201.21
 H       5.008533    -1.607479    -1.698663      23.17
 C       2.822897     0.458560    -2.418473      85.68
 H       2.373350     0.006402    -3.372785      19.54
 C       2.755294     2.139237    -0.701330      32.05
 C       2.143557     3.483499    -0.284221     102.99
 H       2.480292     4.278212    -0.883425      18.60
 O       2.796770     4.016599     0.924730     236.36
 H       3.912224     4.054166     0.974676      24.34
 C       0.480412     3.696340    -0.054530      61.08
 H      -0.000031     3.709184    -1.090959      17.11
 C       0.090647     5.076327     0.407840      89.16
 O       0.155699     5.994353    -0.880455     226.14
 H       0.150913     5.483418    -1.665777      30.05
 H       0.627607     5.474886     1.443674      22.05
 H      -0.973031     5.125922     0.733898      23.30
 C      -1.059585    -0.669865    -0.074613      49.87
 H      -0.526786    -1.661848    -0.468162      16.47
 C      -3.114731     0.633077     0.165607      47.16
 H      -4.160911     0.714208     0.218276      19.11
 C      -2.268271     1.745337     0.535964       0.17
 O      -2.561193     3.115572     0.386777     163.97
 C      -4.000125     3.589655    -0.001033     101.71
 H      -4.377372     2.834819    -0.707782      25.11
 H      -4.836062     3.062205     0.780970      23.41
 H      -3.955027     4.666896    -0.401653      24.34
 C      -0.822058     1.683023     0.778660      -7.16
 O       0.217940     2.712726     1.071627     127.31
 C      -0.210112     0.393641     0.329541      28.24
 H       0.950906     0.447126     0.595591      13.07
 C      -2.499266    -0.538282    -0.144950      20.31
 C      -3.551554    -1.657443    -0.678167      70.57
 H      -4.340913    -1.349823    -1.311010      21.50
 O      -2.820795    -2.637065    -1.502020     281.76
 H      -3.281792    -3.510087    -1.313038      19.03
 C      -4.235108    -2.225458     0.731951     100.25
 H      -3.384898    -2.693544     1.159822      21.54
 O      -4.961074    -1.322647     1.513529     308.06
 H      -4.676762    -1.028695     2.574069      21.93
 C      -5.322209    -3.476018     0.656546      79.82
 O      -5.008740    -4.666071    -0.175994     326.50
 H      -4.289972    -5.124870     0.202073      31.63
 H      -6.240141    -2.921706     0.142774      27.33
 H      -5.670974    -3.550450     1.736046      27.59
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name = lig-etoh-frame_411
 C       2.267432     1.599469    -1.978650      35.26
 H       1.729578     2.283213    -2.606777      23.11
 C       3.686154     1.357252    -0.001100      71.93
 H       4.079616     1.656802     0.946608      12.47
 C       4.003127     0.013188    -0.455333      23.28
 O       4.690089    -0.792964     0.498799     299.04
 C       5.748006    -0.485653     1.379534     110.86
 H       5.444685    -0.675741     2.455776      27.03
 H       5.985972     0.566847     1.221677      28.81
 H       6.539706    -1.169403     1.234579      25.63
 C       3.667799    -0.476553    -1.704068      21.75
 O       4.157046    -1.536317    -2.315736     202.81
 H       4.902962    -1.606474    -1.733678      22.23
 C       2.789203     0.417092    -2.535279      63.22
 H       2.548437     0.033441    -3.484460      20.23
 C       2.677969     2.086240    -0.694637     100.12
 C       2.124289     3.451467    -0.236402     110.80
 H       2.598507     4.369917    -0.892898      17.59
 O       2.849817     4.045770     0.920435     245.00
 H       3.777477     3.918709     0.780292      30.34
 C       0.567179     3.670804    -0.052873      57.01
 H      -0.236272     3.364046    -0.848650      17.81
 C       0.141633     5.087045     0.420578     106.69
 O       0.207959     5.950298    -0.824574     232.43
 H       0.144542     5.365328    -1.710730      26.20
 H       0.626777     5.632152     1.115541      26.12
 H      -0.909512     4.927722     0.694372      23.66
 C      -1.020212    -0.697284    -0.044375      49.66
 H      -0.703503    -1.656371    -0.542219      17.77
 C      -3.077081     0.681184     0.193022      59.98
 H      -4.193360     0.884263     0.344109      20.36
 C      -2.253925     1.822046     0.535062      12.91
 O      -2.634625     3.080903     0.462534     203.38
 C      -4.010360     3.515221    -0.042844     111.82
 H      -4.193114     2.886398    -0.973806      26.05
 H      -4.591431     3.412573     0.775255      29.19
 H      -4.221490     4.516818    -0.467126      26.26
 C      -0.818562     1.642256     0.654819       4.05
 O       0.185273     2.772614     1.078497     129.62
 C      -0.198309     0.356107     0.385156      30.44
 H       0.818061     0.301666     0.360753      15.66
 C      -2.508127    -0.577613    -0.206541      33.39
 C      -3.462346    -1.674227    -0.687380      69.68
 H      -4.444358    -1.316313    -1.264428      20.58
 O      -2.875602    -2.635252    -1.522095     321.90
 H      -3.164636    -3.509501    -1.424385      23.82
 C      -4.241930    -2.228783     0.818984      74.50
 H      -3.340575    -2.694768     1.378966      18.70
 O      -5.007510    -1.325998     1.516952     326.14
 H      -4.810471    -1.284788     2.382713      31.45
 C      -5.387152    -3.386270     0.674344      88.14
 O      -5.040355    -4.676880    -0.165524     270.46
 H      -4.116569    -5.035715     0.143846      24.73
 H      -6.060043    -3.104760    -0.080494      27.12
 H      -5.423030    -3.752676     1.719355      28.04
55
name = lig-etoh-frame_412
 C       2.218056     1.562489    -2.022474      82.89
 H       1.725320     2.254007    -2.749936      17.26
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 C       3.705212     1.425428    -0.002929     105.73
 H       4.166402     1.922138     0.898623      11.17
 C       4.030664     0.031872    -0.432321      -3.42
 O       4.684346    -0.795299     0.519336     280.89
 C       5.766035    -0.453580     1.458986      79.53
 H       5.203972    -0.619672     2.404830      25.52
 H       6.057026     0.603901     1.321095      27.35
 H       6.654004    -1.112652     1.044594      25.32
 C       3.632323    -0.368622    -1.752773      14.43
 O       4.153122    -1.590803    -2.311364     137.84
 H       5.088801    -2.186076    -1.894976      16.92
 C       2.770858     0.348285    -2.596598      18.99
 H       2.710957     0.125007    -3.774744      24.33
 C       2.609733     2.038657    -0.690466      81.26
 C       2.154057     3.492100    -0.220439      94.43
 H       2.260765     3.967071    -1.222813      23.05
 O       2.851807     4.054209     0.943515     226.06
 H       3.856990     3.863264     0.588283      26.01
 C       0.659173     3.626394    -0.009959      61.47
 H      -0.024196     3.081668    -0.699527      18.17
 C       0.166208     5.091971     0.347229      98.14
 O       0.270525     5.912137    -0.756970     222.58
 H      -0.070306     5.356980    -1.628412      24.55
 H       0.893743     5.758695     1.037923      23.05
 H      -0.864191     4.838721     0.703525      22.36
 C      -1.061216    -0.738598    -0.045807      38.19
 H      -0.666424    -1.667708    -0.440923      17.01
 C      -3.032743     0.743013     0.229120      52.69
 H      -4.075906     0.897925     0.279502      17.32
 C      -2.193036     1.839906     0.503449       2.98
 O      -2.738791     3.129919     0.537420     204.20
 C      -3.998240     3.391030    -0.099083     106.66
 H      -4.179628     2.843519    -0.991771      25.97
 H      -4.703885     3.652864     0.914534      22.09
 H      -4.032049     4.509324    -0.373056      24.64
 C      -0.764524     1.604830     0.547987      18.19
 O       0.104950     2.785445     1.078520     125.77
 C      -0.236661     0.348107     0.442536      34.72
 H       0.899578     0.100466     0.162719      14.60
 C      -2.482157    -0.582292    -0.250706      26.49
 C      -3.447224    -1.672359    -0.637164      72.22
 H      -4.227563    -1.138784    -1.078890      22.00
 O      -2.906636    -2.640315    -1.542469     265.34
 H      -3.301018    -3.642213    -1.389831      18.09
 C      -4.223973    -2.318331     0.860254      74.32
 H      -3.486781    -2.540622     1.578257      21.30
 O      -5.068696    -1.292723     1.505450     263.97
 H      -4.679467    -1.420040     2.514123      23.14
 C      -5.358623    -3.338103     0.645001      87.62
 O      -5.051881    -4.676853    -0.143857     269.22
 H      -4.096307    -4.850271     0.193824      25.47
 H      -6.313117    -3.066589    -0.021375      25.01
 H      -5.584531    -3.857898     1.593705      26.47
55
name = lig-etoh-frame_413
 C       2.194210     1.517083    -2.068940      74.74
 H       1.605101     2.162347    -2.730324      17.68
 C       3.680944     1.435229    -0.032664      41.45
 H       4.157358     2.009509     0.807998      10.89
 C       4.066074     0.126862    -0.366772      -1.54
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 O       4.663084    -0.819343     0.498263     247.17
 C       5.768348    -0.404429     1.492255     115.21
 H       5.338455    -0.628709     2.461782      28.00
 H       6.150666     0.640091     1.531640      28.66
 H       6.592723    -0.991245     1.273858      28.30
 C       3.649601    -0.330337    -1.786701      14.86
 O       4.160233    -1.658490    -2.303386     244.77
 H       4.784816    -2.244596    -2.156668      25.72
 C       2.748560     0.331909    -2.642425      33.98
 H       2.798435     0.207795    -3.634170      28.95
 C       2.574579     2.009552    -0.699647      67.49
 C       2.170120     3.499078    -0.242713      78.30
 H       2.110776     3.927152    -1.368083      22.51
 O       2.841908     4.041580     0.926259     218.42
 H       3.890983     4.111327     0.836080      26.80
 C       0.713881     3.570624     0.063112      72.97
 H       0.387294     3.245112    -1.056676      15.94
 C       0.212478     5.065876     0.296242     120.35
 O       0.315744     5.898858    -0.751017     325.29
 H      -0.139329     5.555541    -1.478672      31.81
 H       0.855793     5.378780     1.083797      26.73
 H      -0.774972     5.030206     0.787861      24.50
 C      -1.143019    -0.763663    -0.060529      43.62
 H      -0.451872    -1.745365    -0.216300      16.61
 C      -2.963550     0.751944     0.229766      33.57
 H      -4.078821     0.863308     0.174105      15.05
 C      -2.133787     1.836514     0.447719      -6.55
 O      -2.808186     3.180520     0.618189     191.66
 C      -4.010680     3.345925    -0.090279     118.31
 H      -4.377981     2.598692    -0.893449      24.55
 H      -4.865724     3.333859     0.473340      27.20
 H      -3.608082     4.336198    -0.405255      22.72
 C      -0.694885     1.649683     0.505831      16.56
 O       0.006747     2.745379     1.089241     186.56
 C      -0.255688     0.287160     0.435576      31.26
 H       0.759598     0.138146     0.327782      17.93
 C      -2.436869    -0.532377    -0.230109      33.00
 C      -3.468319    -1.673064    -0.526550      51.80
 H      -4.293695    -0.984836    -1.046141      19.07
 O      -2.935942    -2.670456    -1.552002     272.93
 H      -3.515219    -3.409138    -1.323417      20.44
 C      -4.232126    -2.380398     0.841537      83.80
 H      -3.481644    -2.627214     1.662657      19.91
 O      -5.110132    -1.257644     1.510022     242.26
 H      -4.606795    -1.196532     2.475053      21.31
 C      -5.335645    -3.374748     0.578211     104.03
 O      -5.033161    -4.649886    -0.118679     319.24
 H      -4.209113    -4.876449     0.253619      32.06
 H      -6.229263    -2.839897     0.367288      28.25
 H      -5.880280    -3.656499     1.534821      26.82
55
name = lig-etoh-frame_415
 C       2.164729     1.500084    -2.049350      44.80
 H       1.304262     1.969596    -2.582698      19.40
 C       3.566926     1.423971    -0.059378      56.99
 H       3.883753     1.841612     1.000539       8.97
 C       4.103802     0.130152    -0.454699      77.04
 O       4.699504    -0.789853     0.464487     273.23
 C       5.712430    -0.346918     1.549965     121.13
 H       5.348109    -0.593838     2.520681      29.10
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 H       5.842489     0.750714     1.414490      32.14
 H       6.578821    -0.902064     1.331095      25.82
 C       3.815294    -0.434810    -1.723579      61.70
 O       4.052699    -1.661068    -2.309112     201.37
 H       4.887905    -1.810027    -1.875006      25.87
 C       2.826242     0.350737    -2.578407      71.95
 H       2.526555    -0.010484    -3.504697      19.40
 C       2.590617     2.042448    -0.846062      32.75
 C       2.213004     3.412851    -0.275918      97.22
 H       2.468581     4.387620    -0.894645      16.15
 O       2.812683     4.017989     0.892079     204.64
 H       3.937268     4.027193     0.660447      23.12
 C       0.642052     3.527702     0.015593      62.12
 H       0.022531     3.323530    -1.005052      15.31
 C       0.280190     4.911046     0.404222      92.58
 O       0.440014     5.971157    -0.815506     170.44
 H      -0.061258     5.652051    -1.528535      28.91
 H       0.967131     5.399296     1.119052      24.62
 H      -0.777745     4.983436     0.647897      23.63
 C      -1.048072    -0.775841    -0.019991      31.68
 H      -0.882985    -2.013130    -0.083425      16.89
 C      -2.899178     0.753094     0.119121      25.55
 H      -3.966240     0.881945     0.193421      15.39
 C      -2.099847     1.905938     0.367857      -1.95
 O      -2.800654     3.093658     0.797684     173.08
 C      -4.065017     3.283504    -0.132706      76.96
 H      -3.794453     2.489003    -0.890180      22.73
 H      -4.867965     3.269544     0.588918      24.45
 H      -4.416902     4.235419    -0.776418      23.38
 C      -0.762457     1.629070     0.521055      13.18
 O      -0.046316     2.683313     1.059714     201.77
 C      -0.247116     0.293863     0.340713      52.41
 H       0.659655     0.020837     0.871725      13.15
 C      -2.517710    -0.556034    -0.104637      43.15
 C      -3.573926    -1.639109    -0.352416      74.30
 H      -4.542206    -1.303944    -0.939751      20.01
 O      -3.046468    -2.671820    -1.441794     222.06
 H      -3.812830    -3.414102    -1.639885      19.40
 C      -4.238534    -2.324351     0.810687      91.08
 H      -3.471536    -2.892003     1.385260      18.74
 O      -5.091563    -1.256126     1.488325     276.78
 H      -4.474067    -0.643707     2.242083      20.36
 C      -5.382328    -3.402205     0.567772      93.24
 O      -4.981662    -4.576766    -0.111702     327.29
 H      -4.399208    -5.091423     0.480723      29.27
 H      -5.952237    -3.041005    -0.279037      29.34
 H      -5.644114    -3.612844     1.623595      27.83
55
name = lig-etoh-frame_416
 C       2.153884     1.491638    -2.054768     131.89
 H       1.328730     1.884609    -2.592961      26.34
 C       3.529171     1.365465    -0.055229      73.03
 H       3.652469     1.707032     0.895016      19.74
 C       4.125384     0.060183    -0.511548      20.08
 O       4.749973    -0.755540     0.468814     271.51
 C       5.652936    -0.326638     1.534494      83.71
 H       5.055177    -0.507927     2.508210      24.86
 H       5.752011     0.746053     1.358464      29.37
 H       6.661023    -0.781086     1.202956      23.10
 C       3.784943    -0.411210    -1.754089      42.24
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 O       4.030142    -1.644869    -2.277936     226.75
 H       4.922330    -1.865760    -1.847077      24.44
 C       2.909456     0.348569    -2.474324      69.47
 H       2.362802    -0.227046    -3.335994      17.44
 C       2.657816     2.114845    -0.874509       0.83
 C       2.172934     3.424155    -0.281722      85.69
 H       2.387280     4.091520    -1.218006      12.33
 O       2.833493     3.970548     0.906575     284.07
 H       3.716206     3.891472     0.656684      30.62
 C       0.577602     3.524037    -0.099910      55.19
 H      -0.209979     3.122620    -0.665912      16.78
 C       0.287762     4.943520     0.430857      89.63
 O       0.513956     5.991135    -0.798984     129.27
 H       0.099961     5.469264    -1.665297      23.68
 H       0.917107     5.483669     1.075864      24.00
 H      -0.795678     4.799280     0.672372      22.27
 C      -1.086644    -0.822159     0.002778      31.58
 H      -0.756814    -1.775866    -0.022296      19.43
 C      -2.943994     0.783813     0.053091      58.44
 H      -4.046313     0.947019     0.238176      19.51
 C      -2.160719     1.913302     0.348947       2.49
 O      -2.783955     3.042922     0.837650     175.17
 C      -4.078938     3.252892    -0.156891      71.70
 H      -3.844792     2.530265    -0.932376      24.78
 H      -4.777684     3.062579     0.724649      22.95
 H      -4.360703     4.164715    -0.579555      26.06
 C      -0.836706     1.568394     0.537755       0.54
 O       0.019363     2.676804     1.041505     148.80
 C      -0.202992     0.329704     0.322570      48.48
 H       0.702307     0.073492     0.899811      13.21
 C      -2.505849    -0.621306    -0.056676      23.69
 C      -3.660022    -1.657606    -0.371432      78.15
 H      -4.414450    -1.074315    -0.829791      22.80
 O      -3.105954    -2.655340    -1.347865     307.85
 H      -3.756197    -3.250754    -1.623666      24.02
 C      -4.256003    -2.283971     0.841505     102.23
 H      -3.501718    -2.697561     1.551256      19.67
 O      -5.039815    -1.271858     1.473466     392.19
 H      -4.426482    -0.784897     1.985544      30.87
 C      -5.384489    -3.321200     0.556210     101.50
 O      -4.936802    -4.594270    -0.122467     310.71
 H      -4.375428    -5.077204     0.495963      28.34
 H      -6.181222    -3.306467    -0.293231      25.37
 H      -5.873669    -3.662752     1.501754      26.62
55
name = lig-etoh-frame_417
 C       2.199833     1.484108    -2.051266     138.35
 H       1.379764     1.867871    -2.734462      25.39
 C       3.515850     1.253158    -0.094584      41.40
 H       3.610244     1.605423     1.024335      16.02
 C       4.140294     0.061896    -0.467161      30.90
 O       4.789218    -0.751373     0.442312     287.59
 C       5.575009    -0.269842     1.477078     118.76
 H       5.136273    -0.515638     2.406229      28.31
 H       5.764824     0.831335     1.497513      28.76
 H       6.592203    -0.716167     1.495084      25.36
 C       3.753281    -0.390595    -1.778627      36.75
 O       4.038343    -1.637303    -2.236604     163.68
 H       4.887639    -2.326733    -1.989919      22.04
 C       2.877003     0.372588    -2.430426      63.29
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 H       2.427112    -0.334764    -3.134335      20.57
 C       2.726949     2.155772    -0.859157      38.91
 C       2.085823     3.437074    -0.342269      76.78
 H       2.224003     4.023361    -1.377763      14.85
 O       2.814909     3.905640     0.909043     215.31
 H       3.990536     3.819048     0.747671      22.29
 C       0.542576     3.526532    -0.143516      51.40
 H      -0.151573     3.220274    -1.042076      16.39
 C       0.254256     5.011967     0.355092      88.62
 O       0.559802     5.975366    -0.763228     200.94
 H       0.453064     5.458390    -1.686207      26.04
 H       0.923564     5.360213     1.296024      21.68
 H      -0.758580     4.972679     0.794967      22.72
 C      -1.136100    -0.820105     0.042088      49.69
 H      -0.458593    -1.838848     0.003492      15.94
 C      -3.023922     0.755679     0.001807      77.43
 H      -4.056244     0.868787     0.126354      21.12
 C      -2.243188     1.856075     0.350327       0.33
 O      -2.777857     3.027226     0.823744     180.55
 C      -4.075760     3.217255    -0.111644      79.66
 H      -4.146931     2.547972    -0.997833      24.82
 H      -4.874359     2.660210     0.503220      22.95
 H      -4.024870     4.395477    -0.298188      22.68
 C      -0.813339     1.573152     0.575583      -9.81
 O       0.092570     2.640393     1.035458     158.68
 C      -0.227794     0.309006     0.326525      36.66
 H       0.909567     0.279231     0.639378      10.75
 C      -2.494868    -0.629080    -0.034962      39.26
 C      -3.687564    -1.670558    -0.430600      44.05
 H      -4.416202    -0.847266    -0.849195      20.67
 O      -3.147231    -2.619377    -1.251605     269.75
 H      -3.896334    -3.243674    -1.487913      19.25
 C      -4.315832    -2.271870     0.880153     109.93
 H      -3.577599    -2.608827     1.584689      20.79
 O      -4.999947    -1.267963     1.468979     377.93
 H      -4.312937    -0.797473     2.029049      27.56
 C      -5.397760    -3.319075     0.507070      99.29
 O      -4.886699    -4.619656    -0.128288     292.10
 H      -4.112084    -5.016899     0.516328      23.81
 H      -6.313637    -2.891424     0.048317      28.08
 H      -6.063077    -3.519543     1.370202      26.83
55
name = lig-etoh-frame_418
 C       2.263649     1.550308    -2.028923      91.10
 H       1.573946     1.934421    -2.735511      24.13
 C       3.510610     1.203507    -0.070334       4.06
 H       3.696749     1.421108     0.933866      19.59
 C       4.136029     0.075535    -0.431678      61.75
 O       4.821763    -0.776434     0.381064     297.03
 C       5.531872    -0.179370     1.458054     125.84
 H       5.122024    -0.563605     2.483483      26.52
 H       5.702340     0.897514     1.558336      29.22
 H       6.507128    -0.730250     1.655476      25.31
 C       3.808801    -0.406822    -1.703459      20.88
 O       4.052523    -1.675263    -2.223563     268.02
 H       4.691775    -2.230844    -2.001215      25.39
 C       2.778903     0.346331    -2.467321      73.96
 H       2.391436    -0.257279    -3.300002      21.61
 C       2.746832     2.124950    -0.860889      64.70
 C       2.035404     3.433563    -0.415220     102.01
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 H       2.135314     4.287358    -1.200890      19.91
 O       2.800974     3.837256     0.878532     303.71
 H       3.677580     3.860788     0.806925      31.36
 C       0.506724     3.536979    -0.138460      74.63
 H       0.282642     3.502423    -1.218013      16.60
 C       0.225115     5.071107     0.269970     119.09
 O       0.600345     5.949012    -0.716910     281.78
 H       0.568238     5.562577    -1.529461      33.94
 H       0.820225     5.070306     1.106843      25.26
 H      -0.798060     5.324153     0.677461      24.11
 C      -1.107042    -0.814355     0.098461      57.30
 H      -0.591218    -1.758015    -0.053960      18.48
 C      -3.078499     0.678454    -0.025096      51.03
 H      -4.226642     0.716456    -0.101120      19.09
 C      -2.257344     1.754669     0.396451       3.48
 O      -2.803898     3.018298     0.747421     196.94
 C      -4.059014     3.195653    -0.025177     122.14
 H      -4.153112     2.852353    -1.105012      26.57
 H      -4.927483     2.732824     0.379364      27.27
 H      -3.954186     4.223716     0.081471      25.82
 C      -0.768231     1.608550     0.609001      14.46
 O       0.148774     2.591960     1.003612     197.00
 C      -0.286071     0.295539     0.349527      28.65
 H       0.771851     0.301057     0.217355      15.20
 C      -2.538525    -0.606640    -0.051138      46.94
 C      -3.668481    -1.612746    -0.432672      57.88
 H      -4.455490    -1.074521    -0.953143      23.21
 O      -3.179205    -2.612574    -1.202741     243.51
 H      -3.944501    -3.361852    -1.260562      16.65
 C      -4.372143    -2.295268     0.860079      88.54
 H      -3.532035    -2.810347     1.460680      18.51
 O      -4.995105    -1.207093     1.502129     341.21
 H      -4.288038    -0.786046     2.283819      21.25
 C      -5.432026    -3.360178     0.480555      86.40
 O      -4.842606    -4.621248    -0.118738     331.28
 H      -4.047812    -4.722619     0.374189      32.18
 H      -6.057513    -2.534803    -0.029095      27.18
 H      -5.921545    -3.549504     1.474203      27.03
55
name = lig-etoh-frame_419
 C       2.333165     1.608500    -2.058133      39.92
 H       1.652309     2.251077    -2.696947      15.83
 C       3.496237     1.252966     0.007563       0.47
 H       3.759682     1.494459     1.071942      12.41
 C       4.124989     0.045873    -0.445465      20.33
 O       4.872129    -0.804917     0.325922     274.47
 C       5.514792    -0.126087     1.522816     102.21
 H       4.896080    -0.394846     2.358002      27.63
 H       5.581629     0.966165     1.409391      28.10
 H       6.514748    -0.658621     1.494188      24.85
 C       3.815418    -0.435892    -1.680542      31.75
 O       4.039785    -1.698614    -2.231047     194.44
 H       4.921297    -2.198013    -1.733006      19.41
 C       2.728647     0.249411    -2.489000      83.36
 H       2.365834     0.016376    -3.596629      27.83
 C       2.719161     2.078544    -0.849259      40.73
 C       2.064597     3.440231    -0.413008     107.35
 H       2.254339     4.411837    -1.081509      19.46
 O       2.715063     3.775163     0.840391     212.43
 H       3.873187     3.906670     0.627452      23.38
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 C       0.506480     3.570908    -0.127565      61.85
 H       0.193708     3.362325    -1.199907      16.11
 C       0.166006     5.063841     0.229024     107.60
 O       0.661842     5.965953    -0.679279     171.64
 H       0.465309     5.565871    -1.735685      25.23
 H       0.952614     5.079951     1.153142      23.13
 H      -0.857880     5.446378     0.388662      23.47
 C      -1.122675    -0.797503     0.143972      46.63
 H      -0.772261    -1.849809    -0.134748      16.96
 C      -3.116933     0.623172    -0.020022      44.02
 H      -4.116805     0.720264    -0.326832      17.82
 C      -2.216970     1.678862     0.480681       7.06
 O      -2.830922     2.969567     0.637784     201.20
 C      -4.026148     3.208848     0.053957     113.22
 H      -3.848325     3.224858    -1.039992      24.84
 H      -5.017618     2.796183     0.598636      24.15
 H      -4.300791     4.365794     0.277289      24.21
 C      -0.791779     1.608760     0.624377      26.98
 O       0.183185     2.561020     0.929683     204.16
 C      -0.336575     0.311600     0.377319      37.27
 H       0.715448     0.120665    -0.158651      12.08
 C      -2.578371    -0.608338    -0.090920      43.01
 C      -3.650248    -1.562087    -0.373529      77.71
 H      -4.549377    -1.183102    -1.045286      20.46
 O      -3.190071    -2.666280    -1.207186     283.97
 H      -3.727943    -3.389283    -1.089045      20.38
 C      -4.360147    -2.312109     0.821985      74.97
 H      -3.605580    -2.875141     1.308984      20.41
 O      -4.998846    -1.128457     1.579533     372.81
 H      -4.494882    -1.006079     2.289948      31.08
 C      -5.455970    -3.368867     0.491212      90.01
 O      -4.826021    -4.582632    -0.114451     314.27
 H      -3.897075    -4.563464     0.339341      26.58
 H      -5.904756    -2.877018    -0.407876      27.29
 H      -5.832334    -3.711349     1.442968      27.50
55
name = lig-etoh-frame_420
 C       2.395351     1.594037    -2.157519      38.22
 H       1.841940     2.395214    -2.640919      14.55
 C       3.503031     1.307229     0.093485      23.70
 H       3.688294     1.743774     1.115524      13.34
 C       4.090365     0.037471    -0.440485      -7.06
 O       4.941908    -0.818193     0.295647     222.45
 C       5.499230    -0.104537     1.558917      89.71
 H       4.711259    -0.218437     2.371665      25.47
 H       5.541717     0.957903     1.227920      27.03
 H       6.503697    -0.470330     1.537011      26.01
 C       3.706176    -0.474723    -1.777374      17.70
 O       4.062254    -1.733043    -2.220052     214.02
 H       4.863578    -1.998037    -1.634612      21.74
 C       2.714760     0.219556    -2.499271      79.46
 H       2.537844     0.082132    -3.499931      29.28
 C       2.667265     2.059621    -0.798665      28.50
 C       2.124622     3.456956    -0.365183     111.23
 H       2.482440     4.236420    -1.167592      21.19
 O       2.664657     3.734025     0.819757     306.73
 H       3.550747     3.891556     0.622537      30.41
 C       0.521028     3.579847    -0.169638      63.29
 H      -0.190156     3.103154    -0.908113      17.99
 C       0.133894     5.017565     0.259763     107.85
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 O       0.742782     6.002447    -0.720927     205.40
 H       0.286974     5.786545    -1.513849      30.96
 H       0.611331     5.363529     1.109350      26.79
 H      -0.967475     5.158785     0.332311      25.23
 C      -1.224848    -0.802649     0.164863      39.46
 H      -0.849667    -1.863178    -0.215331      15.95
 C      -3.092533     0.645657     0.018511      62.46
 H      -4.084565     0.945074    -0.431421      18.12
 C      -2.230010     1.657813     0.544604      17.38
 O      -2.796789     2.905779     0.565919     235.20
 C      -4.055085     3.306680     0.121939     127.82
 H      -3.876382     3.395373    -0.994629      25.25
 H      -4.704664     2.611439     0.555575      27.41
 H      -4.461360     4.226973     0.404257      27.28
 C      -0.843704     1.578943     0.631048      20.09
 O       0.195586     2.553368     0.842830     200.88
 C      -0.328396     0.289020     0.358522      30.98
 H       0.587257     0.121560    -0.015669      16.33
 C      -2.576632    -0.636862    -0.113560      43.37
 C      -3.682091    -1.613644    -0.353780      88.23
 H      -4.437783    -1.049867    -0.904550      22.36
 O      -3.157799    -2.722825    -1.238734     248.23
 H      -3.676441    -3.604423    -0.967895      14.88
 C      -4.348444    -2.263371     0.806537      64.60
 H      -3.561601    -2.817789     1.455760      19.20
 O      -5.010130    -1.091540     1.637378     284.27
 H      -4.450521    -1.196072     2.594902      22.59
 C      -5.440177    -3.363225     0.463101      90.86
 O      -4.794596    -4.531076    -0.103813     284.18
 H      -3.878397    -4.750582     0.341311      26.91
 H      -6.179096    -3.383209    -0.430066      25.32
 H      -6.097814    -3.705897     1.337264      26.56
55
name = lig-etoh-frame_421
 C       2.457136     1.572900    -2.178503      53.38
 H       1.967204     2.258895    -2.900596      14.84
 C       3.512000     1.321698     0.123049      44.08
 H       3.648398     1.811555     1.048038      13.37
 C       4.024817     0.050326    -0.430595     -24.05
 O       5.011183    -0.806729     0.281031     205.26
 C       5.458057    -0.083690     1.525843      98.02
 H       4.799999    -0.128055     2.404741      27.41
 H       5.580920     0.940323     1.224882      27.76
 H       6.536438    -0.407190     1.937328      25.07
 C       3.573328    -0.506862    -1.824441      13.35
 O       4.091821    -1.755015    -2.201847     227.71
 H       4.798965    -2.014719    -1.661183      24.09
 C       2.717539     0.274916    -2.526145      66.77
 H       2.655747    -0.184265    -3.662728      24.52
 C       2.617715     2.024869    -0.781847      51.25
 C       2.140817     3.424707    -0.394865     100.08
 H       2.556684     4.097719    -1.287708      23.69
 O       2.619755     3.730941     0.874798     233.69
 H       3.726826     3.950296     0.762614      25.28
 C       0.527685     3.547806    -0.228390      62.19
 H      -0.266061     3.275861    -0.942489      19.83
 C       0.112438     4.990451     0.268766      83.31
 O       0.798095     6.031360    -0.757594     128.86
 H       0.154430     5.951600    -1.573389      27.40
 H       0.281112     5.520095     1.306742      24.96
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 H      -1.003687     4.814869     0.267129      24.29
 C      -1.298846    -0.841674     0.151527      51.37
 H      -0.831125    -1.757923    -0.117037      17.58
 C      -3.045353     0.692324     0.062948      63.92
 H      -3.966689     1.083118    -0.340569      20.93
 C      -2.305757     1.671877     0.559724      17.91
 O      -2.710608     2.911177     0.544994     214.28
 C      -4.098522     3.372702     0.153732     109.65
 H      -4.292011     3.404489    -0.933887      26.65
 H      -4.636985     2.307487     0.284451      22.14
 H      -4.354029     4.358404     0.756412      24.69
 C      -0.832701     1.524779     0.629903       4.97
 O       0.184753     2.543562     0.797067     193.11
 C      -0.356707     0.236257     0.332097      26.93
 H       0.873092     0.170873     0.285915      13.17
 C      -2.610152    -0.649621    -0.103544      33.37
 C      -3.688801    -1.710795    -0.399578      69.25
 H      -4.463343    -0.972018    -0.890269      20.85
 O      -3.122316    -2.777150    -1.269704     270.10
 H      -3.609579    -3.629646    -1.014917      15.37
 C      -4.385515    -2.193985     0.853971      82.71
 H      -3.698637    -2.637557     1.508943      21.19
 O      -4.993712    -1.095305     1.693357     318.38
 H      -4.557411    -1.335117     2.623004      24.53
 C      -5.445492    -3.373311     0.418656      96.78
 O      -4.726888    -4.513136    -0.090970     340.03
 H      -4.121436    -4.928982     0.513235      30.85
 H      -6.383192    -3.340430    -0.176537      26.86
 H      -6.120278    -3.508140     1.270157      27.22
55
name = lig-etoh-frame_422
 C       2.478164     1.598795    -2.142306      63.27
 H       2.068413     2.051142    -3.064260      17.18
 C       3.492924     1.280704     0.062442      58.12
 H       3.743438     1.740287     1.112544      12.75
 C       3.953592     0.048262    -0.428852      -5.88
 O       5.059797    -0.763625     0.275671     234.52
 C       5.454751    -0.065226     1.485397     116.96
 H       4.730739    -0.139712     2.349647      26.96
 H       5.666457     1.030368     1.307138      27.21
 H       6.258313    -0.462652     2.018135      26.97
 C       3.514641    -0.545544    -1.724141      -2.62
 O       4.087673    -1.750640    -2.203710     157.23
 H       4.922292    -2.137494    -1.525554      20.43
 C       2.747806     0.292887    -2.640338      65.67
 H       2.595998    -0.133328    -3.517190      24.02
 C       2.597509     1.972757    -0.814021      77.90
 C       2.115379     3.357373    -0.463117      94.11
 H       2.501900     4.113481    -1.287972      24.92
 O       2.612022     3.765790     0.952651     247.04
 H       3.638217     3.922305     0.995604      28.74
 C       0.540904     3.517666    -0.265043      61.04
 H       0.062325     3.565116    -1.331305      19.04
 C       0.092164     4.983678     0.244009      89.57
 O       0.803451     6.030821    -0.771781      98.70
 H       0.168495     6.079259    -1.668972      27.14
 H       0.224083     5.276165     1.254936      27.69
 H      -0.971525     4.867352     0.036710      24.54
 C      -1.291246    -0.884500     0.116550      41.28
 H      -0.736800    -2.000213     0.049453      15.91
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 C      -3.049894     0.682396     0.082548      47.46
 H      -4.044531     0.948622    -0.271614      22.38
 C      -2.279694     1.705867     0.557354       6.55
 O      -2.647285     3.029640     0.531533     181.73
 C      -4.133786     3.370169     0.189449     122.27
 H      -4.479407     3.682603    -0.858224      26.34
 H      -4.767918     2.580060     0.324708      28.83
 H      -4.188921     4.075262     0.975576      27.19
 C      -0.802014     1.466264     0.610544       9.78
 O       0.151299     2.520613     0.788817     183.48
 C      -0.364175     0.190470     0.326032      49.66
 H       0.602416     0.076981     0.609897      17.64
 C      -2.686087    -0.653223    -0.078745      28.38
 C      -3.669896    -1.754071    -0.478936      68.27
 H      -4.501656    -1.273528    -1.056757      21.15
 O      -3.093655    -2.812505    -1.290294     289.27
 H      -3.575754    -3.611978    -1.088016      18.18
 C      -4.472265    -2.145639     0.903019      74.07
 H      -3.701946    -2.729268     1.526990      17.05
 O      -4.974494    -1.126212     1.727384     387.04
 H      -4.629746    -1.267637     2.546420      30.04
 C      -5.472610    -3.365482     0.423002      74.90
 O      -4.660752    -4.514398    -0.082207     291.13
 H      -4.424205    -5.014332     0.846512      24.26
 H      -6.229637    -2.929088    -0.291360      28.07
 H      -5.837765    -3.548815     1.499131      27.48
55
name = lig-etoh-frame_423
 C       2.461879     1.578586    -2.176838      47.54
 H       2.011050     2.277658    -2.890450      19.21
 C       3.450687     1.221762    -0.011130      54.31
 H       3.770104     1.529885     0.888646      16.76
 C       3.920634    -0.008384    -0.428894      13.54
 O       5.073570    -0.690816     0.259292     236.34
 C       5.441395    -0.029575     1.470774     105.98
 H       4.489074    -0.097220     2.073925      25.34
 H       5.777815     0.997060     1.392281      27.97
 H       6.297986    -0.773282     1.898059      23.76
 C       3.499774    -0.572021    -1.607722      35.11
 O       4.078838    -1.734622    -2.187913     230.81
 H       4.723065    -2.094504    -1.618689      28.74
 C       2.836110     0.277770    -2.656831      71.48
 H       2.421980    -0.035650    -3.784997      18.13
 C       2.607182     1.953086    -0.843801      27.38
 C       2.082963     3.317192    -0.458009      95.32
 H       2.400808     4.152753    -1.204106      22.18
 O       2.595428     3.802807     1.007722     255.63
 H       3.587483     3.903674     0.954178      28.44
 C       0.570899     3.514330    -0.306306      63.45
 H       0.457274     3.465649    -1.391889      16.49
 C       0.085471     4.961936     0.139755      93.60
 O       0.769121     6.011237    -0.764792     193.47
 H       0.329731     5.965881    -1.528378      34.07
 H       0.387826     5.083592     1.235176      24.32
 H      -0.988091     5.194784    -0.167655      23.02
 C      -1.254340    -0.956782     0.077820      44.90
 H      -0.967089    -1.895557     0.149976      21.51
 C      -3.115256     0.657633     0.087327      59.10
 H      -4.214060     0.766125    -0.142252      20.84
 C      -2.167941     1.755510     0.522057      -9.40
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 O      -2.620975     3.168831     0.503201     152.35
 C      -4.132107     3.369088     0.236837     114.04
 H      -4.227262     4.034044    -0.635031      25.56
 H      -4.928721     2.599442     0.608919      24.84
 H      -4.318132     4.048574     1.148795      26.43
 C      -0.812694     1.458866     0.569462      22.13
 O       0.102702     2.496559     0.778975     171.11
 C      -0.396130     0.123057     0.355220      42.33
 H       0.671512    -0.201004     0.761541      15.68
 C      -2.701054    -0.681213    -0.066835      30.76
 C      -3.671776    -1.752480    -0.533824      54.98
 H      -4.522746    -1.462664    -1.309796      19.18
 O      -3.056959    -2.827680    -1.299047     243.73
 H      -3.606393    -3.734418    -1.069359      14.27
 C      -4.501334    -2.188797     0.916045      79.78
 H      -3.751006    -2.794486     1.377216      17.66
 O      -4.984817    -1.149210     1.721151     326.20
 H      -4.448256    -1.148658     2.744027      21.10
 C      -5.484199    -3.315753     0.490744      79.12
 O      -4.627476    -4.512451    -0.048544     275.87
 H      -4.566131    -5.001234     0.784618      27.50
 H      -5.943100    -2.803191    -0.372627      27.80
 H      -5.809076    -3.779900     1.403319      27.33
55
name = lig-etoh-frame_424
 C       2.425213     1.528340    -2.257349      47.35
 H       1.934125     2.438470    -2.675011      17.13
 C       3.396530     1.154985    -0.077373      38.02
 H       3.790457     1.581551     0.947633      16.34
 C       3.945255    -0.094737    -0.401742      28.13
 O       5.053747    -0.603783     0.203820     248.96
 C       5.429273    -0.038293     1.484671     116.78
 H       4.481773     0.024431     2.010692      26.56
 H       5.937949     0.970981     1.419241      27.43
 H       6.098333    -0.746288     1.748854      26.91
 C       3.495944    -0.606557    -1.620506      37.14
 O       4.044806    -1.708610    -2.168938     227.37
 H       4.721292    -2.161541    -1.565766      24.40
 C       2.909576     0.267885    -2.619872      58.71
 H       2.599569     0.072332    -3.563330      22.04
 C       2.625680     1.969831    -0.870101      38.04
 C       2.075261     3.324765    -0.350341      94.42
 H       2.389029     4.214410    -1.112413      18.09
 O       2.569608     3.827599     1.023871     244.78
 H       3.682485     3.898921     0.760764      23.87
 C       0.603385     3.503734    -0.348372      45.75
 H       0.237725     3.063608    -1.377883      15.59
 C       0.092201     4.947243    -0.005992     106.46
 O       0.740185     5.978098    -0.722776     210.90
 H       0.316425     5.732878    -1.742837      24.89
 H       0.483485     5.030232     1.039407      24.25
 H      -0.930609     5.230817    -0.045313      24.03
 C      -1.276223    -0.977629     0.047292      40.37
 H      -1.029221    -2.222841     0.189585      18.03
 C      -3.163916     0.649416     0.107880      43.72
 H      -4.211615     0.797277     0.063790      20.09
 C      -2.149780     1.797865     0.427195     -19.71
 O      -2.612210     3.255650     0.470547     167.87
 C      -4.099360     3.418888     0.364455     119.96
 H      -4.054919     4.113619    -0.493105      24.67
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 H      -4.684914     2.483359     0.478700      25.69
 H      -4.473468     4.122239     1.132587      27.20
 C      -0.816653     1.475685     0.507815      14.17
 O       0.064132     2.488674     0.756404     176.47
 C      -0.401069     0.024324     0.422444      35.83
 H       0.612499    -0.280522     0.623903      17.03
 C      -2.663491    -0.695074    -0.089157      41.28
 C      -3.712484    -1.743949    -0.561983      64.69
 H      -4.417318    -1.349340    -1.325301      20.77
 O      -3.016928    -2.853423    -1.288429     286.77
 H      -3.453515    -3.627028    -1.016359      19.11
 C      -4.461492    -2.277761     0.891282      84.30
 H      -3.603997    -2.796093     1.424598      18.23
 O      -5.001805    -1.166300     1.730208     363.40
 H      -4.303551    -1.067643     2.366964      27.79
 C      -5.452983    -3.275678     0.550310      90.06
 O      -4.635694    -4.486388    -0.015958     282.80
 H      -4.390813    -5.107149     0.682433      29.21
 H      -6.078886    -3.043531    -0.339217      27.05
 H      -6.261568    -3.804968     1.224894      24.93
55
name = lig-etoh-frame_425
 C       2.386804     1.532399    -2.254061      64.76
 H       1.869907     2.215144    -2.971783      24.72
 C       3.370147     1.109469    -0.065682      67.45
 H       3.625429     1.636847     0.802531      22.29
 C       3.939717    -0.132140    -0.400197      24.93
 O       5.045882    -0.537724     0.141775     228.27
 C       5.406992    -0.038691     1.479705     103.10
 H       4.574590     0.158627     2.263643      25.65
 H       6.018914     0.862631     1.395140      26.27
 H       6.101913    -0.901424     1.972377      24.11
 C       3.515116    -0.618368    -1.689099      34.35
 O       4.015074    -1.722553    -2.165214     177.40
 H       4.751845    -2.266479    -1.521017      21.01
 C       2.945815     0.288344    -2.549336      55.36
 H       2.863064    -0.188163    -3.677439      17.74
 C       2.634138     1.985252    -0.912338      29.02
 C       2.101251     3.365505    -0.227936     101.83
 H       2.471388     4.182783    -1.019733      17.99
 O       2.575708     3.833956     0.990627     311.67
 H       3.444553     3.950099     0.890656      32.06
 C       0.571732     3.438443    -0.413097      62.93
 H      -0.031249     2.856403    -1.072408      20.12
 C       0.110923     4.912193    -0.099278     110.49
 O       0.705114     5.942484    -0.745589     280.82
 H       0.581420     5.764025    -1.710399      29.89
 H       0.452349     5.080284     0.932455      25.18
 H      -1.043448     4.901215     0.115198      22.77
 C      -1.323325    -1.039093     0.048156      52.46
 H      -1.051434    -1.958642     0.020490      20.26
 C      -3.129582     0.663342     0.139504      46.27
 H      -4.243752     0.873948     0.241385      17.38
 C      -2.254533     1.817706     0.298163     -22.77
 O      -2.596916     3.275250     0.452673     199.94
 C      -4.026203     3.507153     0.491175     127.89
 H      -4.273005     3.937683    -0.537122      26.04
 H      -4.437593     2.489196     0.207244      24.01
 H      -4.454632     4.124451     1.308302      25.92
 C      -0.798740     1.456539     0.433529      -7.34
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 O       0.051678     2.504550     0.738472     167.67
 C      -0.408275    -0.024465     0.484123      24.07
 H       0.707706    -0.212341     0.526958      16.49
 C      -2.659451    -0.666475    -0.139633      20.05
 C      -3.722985    -1.750552    -0.547201      61.84
 H      -4.464091    -1.141633    -1.222067      19.78
 O      -2.973525    -2.853010    -1.264360     249.16
 H      -3.433518    -3.725593    -0.891170      14.57
 C      -4.378949    -2.318153     0.864362      88.05
 H      -3.558122    -2.700763     1.469235      21.15
 O      -5.013091    -1.202451     1.701657     331.89
 H      -4.118324    -0.975004     2.248972      21.91
 C      -5.466132    -3.339667     0.569316      84.47
 O      -4.675740    -4.452810     0.014104     293.79
 H      -4.064493    -5.091789     0.643615      26.69
 H      -6.156351    -3.204973    -0.306191      26.13
 H      -6.353824    -3.466721     1.168672      24.98
55
name = lig-etoh-frame_426
 C       2.351660     1.570292    -2.223450      92.78
 H       1.916463     1.844600    -3.204020      21.89
 C       3.331695     1.108465    -0.044570      65.59
 H       3.596369     1.619827     0.926589      20.79
 C       3.857660    -0.088003    -0.451580      22.04
 O       5.087175    -0.519056     0.129782     226.99
 C       5.414996    -0.067624     1.501792     124.98
 H       4.684651     0.200769     2.216547      28.58
 H       6.070165     0.809164     1.351177      26.77
 H       5.904883    -0.803778     2.014408      27.59
 C       3.569048    -0.584377    -1.694846      12.31
 O       4.010990    -1.811638    -2.188516     228.87
 H       4.625662    -2.155275    -1.664906      25.41
 C       2.930446     0.291093    -2.565396      61.85
 H       3.148455    -0.226153    -3.469989      21.42
 C       2.630158     1.991176    -0.920787      56.72
 C       2.129337     3.382525    -0.239613     105.03
 H       2.567989     4.124607    -1.040137      19.57
 O       2.559540     3.825489     0.984595     239.41
 H       3.679214     4.072440     0.994055      23.57
 C       0.519115     3.362441    -0.412522      66.24
 H       0.026139     2.898735    -1.336909      22.13
 C       0.077776     4.815718    -0.093600     101.28
 O       0.687197     5.936540    -0.822754     265.59
 H       0.665202     5.859334    -1.791398      30.59
 H       0.432984     5.053307     0.985072      24.46
 H      -0.969124     4.659915    -0.086895      24.82
 C      -1.362947    -1.025567     0.076449      26.29
 H      -0.914190    -2.185566    -0.231114      15.48
 C      -3.093446     0.714439     0.161386      60.21
 H      -4.139201     0.773193     0.296972      18.18
 C      -2.319087     1.810903     0.183318      -7.00
 O      -2.566825     3.241800     0.444722     208.65
 C      -3.960414     3.585081     0.541168     129.84
 H      -4.488522     4.010349    -0.346194      26.86
 H      -4.480949     2.567530     0.299947      24.04
 H      -4.291891     3.936433     1.562756      26.36
 C      -0.821468     1.410327     0.368103     -17.96
 O       0.049064     2.519630     0.740829     171.26
 C      -0.423082     0.006578     0.510017      33.12
 H       0.716160    -0.108352     0.483111      17.78
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 C      -2.688736    -0.634152    -0.189849      24.05
 C      -3.692090    -1.752903    -0.500564      77.83
 H      -4.557960    -1.244384    -1.033266      20.31
 O      -2.952172    -2.836658    -1.223709     264.01
 H      -3.436047    -3.676911    -0.887314      16.02
 C      -4.338866    -2.292408     0.829141      77.38
 H      -3.539027    -2.766547     1.436758      21.17
 O      -4.994135    -1.260176     1.642503     337.62
 H      -4.213088    -0.804017     2.292265      23.15
 C      -5.482222    -3.417802     0.544004      67.79
 O      -4.714733    -4.470212     0.046335     361.13
 H      -4.050598    -4.669316     0.690479      30.33
 H      -5.957908    -3.052746    -0.382938      27.59
 H      -6.074971    -3.383401     1.576719      24.99
55
name = lig-etoh-frame_427
 C       2.352534     1.548437    -2.232713      89.42
 H       1.859936     1.972766    -3.165704      19.88
 C       3.274744     1.173437    -0.017097      34.45
 H       3.611222     1.424251     1.016115      19.62
 C       3.834436    -0.027032    -0.458031      26.31
 O       5.116155    -0.529436     0.147453     204.60
 C       5.440397    -0.079247     1.502238      98.77
 H       4.458551     0.294218     2.046397      24.29
 H       6.158913     0.783479     1.408130      26.31
 H       5.964686    -1.003430     2.043776      24.26
 C       3.624423    -0.565716    -1.710030      14.98
 O       3.986547    -1.887508    -2.229484     121.24
 H       4.844381    -2.226268    -1.630467      19.90
 C       2.910486     0.276187    -2.581667      65.12
 H       3.059827    -0.050645    -3.716066      24.88
 C       2.604634     2.013522    -0.870254      57.61
 C       2.142819     3.354639    -0.386486      97.93
 H       2.528712     4.175838    -1.154383      21.46
 O       2.570872     3.818108     1.018478     293.21
 H       3.519736     3.997863     0.864990      27.07
 C       0.507938     3.302418    -0.379694      80.45
 H       0.440580     3.175021    -1.488975      19.28
 C       0.039196     4.718017    -0.063588      90.18
 O       0.672869     5.931742    -0.892056     163.54
 H       0.444505     5.751124    -2.007364      24.26
 H       0.300266     4.927374     0.920840      25.53
 H      -1.082861     4.798448    -0.373799      21.87
 C      -1.359341    -0.998560     0.096534      39.73
 H      -1.036147    -1.870838    -0.269055      18.65
 C      -3.123993     0.728068     0.147320      65.35
 H      -4.235635     0.753871     0.289443      17.66
 C      -2.251553     1.824737     0.115919      11.18
 O      -2.533560     3.175448     0.425719     198.76
 C      -3.943584     3.600961     0.573667     122.81
 H      -4.341045     4.481711    -0.045781      25.78
 H      -4.638689     2.697039     0.680313      24.21
 H      -4.026937     3.823838     1.637442      26.84
 C      -0.876847     1.389763     0.330400       6.58
 O       0.032957     2.504144     0.730757     189.53
 C      -0.450416     0.090399     0.480582      49.36
 H       0.584242    -0.097655     0.575784      19.55
 C      -2.690032    -0.619062    -0.207274      17.14
 C      -3.651685    -1.746822    -0.439664      82.60
 H      -4.611637    -1.469972    -1.080546      19.42
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 O      -2.952549    -2.805404    -1.173305     302.21
 H      -3.449684    -3.593467    -1.016635      18.27
 C      -4.331173    -2.263195     0.812627      71.21
 H      -3.554181    -2.875363     1.365312      20.50
 O      -4.964776    -1.303539     1.569272     439.24
 H      -4.482496    -0.981410     2.226368      36.60
 C      -5.463838    -3.400604     0.530039      68.66
 O      -4.747376    -4.541652     0.078574     341.77
 H      -4.034677    -4.474051     0.815966      23.73
 H      -6.056417    -2.883783    -0.258962      27.82
 H      -5.619116    -3.594094     1.573096      28.19
55
name = lig-etoh-frame_428
 C       2.382975     1.499599    -2.239337      47.40
 H       1.875714     2.304575    -2.805329      18.86
 C       3.250761     1.218324     0.031456      42.52
 H       3.507310     1.478950     1.012380      21.68
 C       3.902011     0.011361    -0.428254      24.93
 O       5.108251    -0.545508     0.167730     199.94
 C       5.460994    -0.095502     1.503694     123.06
 H       4.564033     0.200139     1.883029      28.68
 H       6.186369     0.709930     1.548717      28.09
 H       5.852809    -0.953518     1.975762      27.11
 C       3.660153    -0.589422    -1.770615      26.79
 O       3.967565    -1.922762    -2.235926     167.94
 H       4.926974    -2.257468    -1.905938      20.41
 C       2.896146     0.255279    -2.634623      50.72
 H       2.653319     0.254649    -3.720920      23.32
 C       2.558271     2.033821    -0.851992      38.06
 C       2.121212     3.337058    -0.500251      87.17
 H       2.325637     4.278511    -1.196108      18.95
 O       2.570542     3.793561     1.011063     231.99
 H       3.618874     3.938708     0.843030      24.46
 C       0.578171     3.309566    -0.360122      77.96
 H       0.428751     3.097599    -1.434823      17.31
 C      -0.023928     4.677716    -0.091221      90.18
 O       0.649119     5.890822    -0.967950     195.90
 H       0.159331     5.641207    -1.707596      29.11
 H       0.086577     4.944942     1.062259      22.78
 H      -0.992431     4.969365    -0.415772      23.09
 C      -1.352564    -0.887941     0.106223      47.18
 H      -0.961764    -2.000248    -0.246483      16.25
 C      -3.192716     0.712354     0.088188      65.71
 H      -4.257183     0.922664     0.193005      17.04
 C      -2.180100     1.815650     0.099642      20.43
 O      -2.514273     3.102526     0.385634     183.27
 C      -3.931686     3.598861     0.642814     113.98
 H      -3.930738     4.620393     0.282547      25.02
 H      -4.884423     2.918424     0.773902      22.87
 H      -3.665100     3.976336     1.720377      23.75
 C      -0.909512     1.447122     0.321265      28.23
 O       0.004996     2.451128     0.687998     203.81
 C      -0.494579     0.143835     0.407633      46.68
 H       0.603130    -0.114578     0.795452      17.59
 C      -2.677692    -0.591945    -0.177726      24.41
 C      -3.644115    -1.735543    -0.423476      91.13
 H      -4.435107    -1.546102    -1.195105      19.48
 O      -2.944566    -2.770174    -1.117149     262.50
 H      -3.582094    -3.634084    -1.207138      16.51
 C      -4.316926    -2.297691     0.808644      95.36
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 H      -3.558979    -2.820012     1.387769      21.51
 O      -4.970789    -1.317282     1.482935     333.07
 H      -4.445340    -1.201169     2.530590      22.33
 C      -5.387947    -3.322419     0.529764      88.00
 O      -4.770917    -4.632288     0.099719     309.86
 H      -3.945809    -4.754455     0.766623      25.24
 H      -6.380932    -3.016566     0.056021      26.02
 H      -5.792537    -3.711575     1.542087      25.77
55
name = lig-etoh-frame_429
 C       2.420973     1.501863    -2.169377      32.23
 H       1.965878     2.395550    -2.696624      20.67
 C       3.275484     1.209444     0.069390      48.66
 H       3.381332     1.755836     1.111885      18.05
 C       4.003796     0.025897    -0.436003      16.08
 O       5.079599    -0.560517     0.176211     203.48
 C       5.473555    -0.119294     1.488233     108.72
 H       4.504717     0.196939     2.129535      24.34
 H       6.246313     0.729113     1.590387      26.11
 H       5.825761    -1.054991     2.070187      24.88
 C       3.676458    -0.605326    -1.823614      27.03
 O       3.957134    -1.923088    -2.231593     204.43
 H       4.850827    -2.230395    -2.142190      23.88
 C       2.860984     0.262088    -2.700175      50.12
 H       2.457671     0.070840    -3.723338      21.77
 C       2.546232     1.975162    -0.896499      31.90
 C       2.062387     3.383096    -0.493589      90.34
 H       2.227776     4.252918    -1.225706      19.06
 O       2.574822     3.761687     0.944051     230.62
 H       3.669563     3.841892     0.987194      24.69
 C       0.627099     3.348771    -0.377905      60.20
 H       0.055463     2.810515    -1.232577      17.81
 C      -0.057698     4.726895    -0.105501      98.35
 O       0.626748     5.815481    -0.997714     220.61
 H      -0.127290     5.693256    -1.812629      21.65
 H      -0.076111     4.969565     0.888905      25.76
 H      -1.158487     4.790365    -0.384838      21.89
 C      -1.337534    -0.819456     0.071497      65.65
 H      -0.978432    -1.866775     0.131130      20.36
 C      -3.214290     0.728980    -0.005104      55.09
 H      -4.251002     1.046454     0.003649      17.37
 C      -2.248391     1.752212     0.116633      19.98
 O      -2.522987     3.053189     0.327961     203.51
 C      -3.858426     3.626738     0.787418     122.72
 H      -3.756725     4.601696     0.195417      24.87
 H      -4.736476     3.154089     0.607192      27.44
 H      -3.621722     3.944935     1.753738      26.19
 C      -0.867340     1.523823     0.321969      22.79
 O       0.005175     2.406674     0.638883     215.03
 C      -0.476801     0.166911     0.350128      45.61
 H       0.411275     0.020252     0.787131      20.60
 C      -2.715048    -0.558408    -0.124107      36.69
 C      -3.643475    -1.728807    -0.454766      75.68
 H      -4.422166    -1.270241    -1.213396      20.92
 O      -2.918033    -2.776786    -1.073598     296.82
 H      -3.571482    -3.428693    -1.293871      21.72
 C      -4.293174    -2.361007     0.792675      92.59
 H      -3.463010    -2.738737     1.487292      18.85
 O      -4.981805    -1.271828     1.472046     341.52
 H      -4.631921    -1.478295     2.317735      25.77
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 C      -5.337758    -3.324122     0.583281     100.58
 O      -4.792387    -4.716066     0.098369     319.77
 H      -4.092356    -5.086744     0.605881      31.05
 H      -6.334615    -3.250902     0.126562      27.47
 H      -5.949102    -3.500467     1.486927      27.24
55
name = lig-etoh-frame_430
 C       2.438398     1.538703    -2.146290      77.07
 H       2.030138     2.134983    -2.953432      23.75
 C       3.333409     1.175837     0.081130      55.58
 H       3.388460     1.699122     0.949702      20.33
 C       4.067509     0.054179    -0.488653      -2.79
 O       5.061554    -0.586236     0.192161     216.73
 C       5.454474    -0.149375     1.524279     122.96
 H       4.731608     0.174657     2.181648      28.74
 H       6.172899     0.622779     1.438599      27.92
 H       5.886206    -1.042647     2.006195      26.02
 C       3.667075    -0.562888    -1.859447      15.61
 O       3.928838    -1.901467    -2.221938     124.89
 H       5.035703    -2.203565    -2.306008      21.69
 C       2.840350     0.263528    -2.724760      42.16
 H       2.451029    -0.376983    -3.630311      21.60
 C       2.585655     1.904991    -0.877591      36.00
 C       2.048180     3.409441    -0.417447      93.94
 H       2.348584     4.169154    -1.324292      20.65
 O       2.572390     3.730112     0.854811     304.03
 H       3.536789     3.806466     0.812588      28.44
 C       0.536469     3.381977    -0.406705      70.84
 H       0.042176     2.886365    -1.201176      20.91
 C      -0.092360     4.807757    -0.163053     101.78
 O       0.561047     5.718727    -1.009466     301.91
 H       0.209150     5.922286    -1.893281      28.59
 H      -0.010310     5.132588     0.986661      24.15
 H      -1.124759     4.414224    -0.337872      21.73
 C      -1.366101    -0.801892     0.042276      49.92
 H      -1.013889    -1.866437     0.366188      20.27
 C      -3.220720     0.766126    -0.108928      60.03
 H      -4.302855     1.017674    -0.252520      24.17
 C      -2.329174     1.696285     0.163670      11.33
 O      -2.568090     3.045804     0.270018     215.84
 C      -3.702756     3.699823     0.897588     116.98
 H      -3.838600     4.487394     0.171032      25.21
 H      -4.701980     3.127832     0.365193      23.19
 H      -3.804016     3.811689     2.092268      23.79
 C      -0.865214     1.508577     0.293645      12.42
 O       0.074560     2.431584     0.639605     192.89
 C      -0.432232     0.230221     0.306550      28.41
 H       0.662332     0.029061     0.758316      17.93
 C      -2.758440    -0.564700    -0.080385      35.66
 C      -3.651201    -1.710814    -0.492550      75.07
 H      -4.431525    -1.111243    -1.034693      21.16
 O      -2.873003    -2.793139    -1.054638     273.14
 H      -3.564943    -3.420925    -1.345655      20.12
 C      -4.258334    -2.356536     0.774729      97.80
 H      -3.470003    -2.703540     1.384835      19.50
 O      -4.999314    -1.220474     1.469871     310.77
 H      -4.784651    -1.405632     2.455675      25.01
 C      -5.337001    -3.464051     0.653949      67.50
 O      -4.848040    -4.769975     0.072612     297.80
 H      -4.154604    -5.297447     0.742184      23.76
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 H      -5.987072    -3.182290    -0.296309      26.18
 H      -5.745403    -3.379276     1.722060      27.76
55
name = lig-etoh-frame_431
 C       2.435861     1.530245    -2.243903      74.50
 H       1.926893     2.055220    -3.125529      20.25
 C       3.408369     1.110711     0.018495      54.50
 H       3.623893     1.521824     1.106762      19.04
 C       4.090659     0.079854    -0.557013      12.23
 O       5.048256    -0.632995     0.213512     224.36
 C       5.453278    -0.193536     1.551004     104.80
 H       4.611656     0.242539     2.266738      23.43
 H       6.229018     0.641510     1.281838      25.79
 H       6.023249    -1.067929     1.929025      24.72
 C       3.660833    -0.481062    -1.861185      37.42
 O       3.924942    -1.873136    -2.215211     216.97
 H       4.802917    -2.028863    -2.231124      28.12
 C       2.848878     0.216146    -2.679228      42.15
 H       2.513255    -0.364853    -3.465952      23.72
 C       2.623472     1.912417    -0.802786      65.74
 C       2.060789     3.358782    -0.394218      94.11
 H       2.476728     4.031068    -1.194337      22.87
 O       2.551104     3.713322     0.787623     248.35
 H       3.657073     3.891376     0.502355      22.40
 C       0.427131     3.419196    -0.404597      61.23
 H       0.224893     3.159689    -1.572116      19.02
 C      -0.142321     4.830192    -0.193688     122.38
 O       0.515238     5.670518    -1.014332     327.76
 H       0.298640     5.778758    -1.967437      28.72
 H       0.108662     5.224185     0.739019      26.52
 H      -1.182618     4.589595    -0.348763      24.09
 C      -1.393488    -0.808019     0.051476      44.19
 H      -1.107539    -1.889032     0.445637      19.18
 C      -3.272391     0.752113    -0.215722      38.37
 H      -4.286103     0.937736    -0.466024      23.20
 C      -2.317896     1.728692     0.233812       7.88
 O      -2.613899     3.076230     0.224144     248.55
 C      -3.614040     3.726684     0.941928     136.50
 H      -3.814625     4.770421     0.500910      26.06
 H      -4.420771     3.173140     0.654080      27.38
 H      -3.866107     3.673832     1.935347      27.99
 C      -0.903341     1.483786     0.268486       0.13
 O       0.150393     2.491123     0.671318     146.43
 C      -0.364799     0.235698     0.280226      40.71
 H       0.635009     0.030202     0.421941      20.23
 C      -2.761559    -0.589966    -0.075939      26.78
 C      -3.660049    -1.693772    -0.477953      73.69
 H      -4.540318    -1.302635    -1.141120      21.88
 O      -2.833715    -2.804066    -1.066116     224.01
 H      -3.493779    -3.580066    -1.380553      19.67
 C      -4.254875    -2.305553     0.775726      81.48
 H      -3.339008    -2.698474     1.362375      19.00
 O      -5.004653    -1.193767     1.462757     278.10
 H      -4.960183    -1.099870     2.583070      24.07
 C      -5.331533    -3.610906     0.666247      88.08
 O      -4.906232    -4.825518     0.070424     346.63
 H      -4.345805    -5.146142     0.760228      29.78
 H      -5.670091    -3.090634    -0.175008      28.48
 H      -5.687745    -3.565652     1.698051      28.70
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name = lig-etoh-frame_432
 C       2.424763     1.500984    -2.323889      27.51
 H       1.826620     2.147273    -2.909040      18.33
 C       3.478507     1.102622    -0.028112      38.15
 H       3.821642     1.185003     0.954855      21.73
 C       4.130370     0.040526    -0.613175      15.99
 O       5.021561    -0.699190     0.221226     224.59
 C       5.470283    -0.206022     1.546400     115.68
 H       4.672711     0.083620     2.165526      27.47
 H       6.125004     0.597570     1.419784      28.89
 H       6.078368    -1.075756     1.960955      25.28
 C       3.713433    -0.462347    -1.803124      37.98
 O       3.899419    -1.813440    -2.202515     184.76
 H       4.958710    -2.014307    -2.067834      22.76
 C       2.841225     0.212440    -2.610424      43.52
 H       2.459846    -0.238218    -3.663767      23.31
 C       2.617823     1.953637    -0.829686      67.57
 C       2.033685     3.254278    -0.451402      99.36
 H       2.554933     4.025740    -1.252754      22.26
 O       2.583047     3.732727     0.776162     298.03
 H       3.443257     3.936091     0.698107      32.66
 C       0.400948     3.444817    -0.427516      75.62
 H       0.309382     3.312404    -1.464241      19.67
 C      -0.211546     4.792213    -0.197892      98.74
 O       0.511161     5.701810    -1.055671     277.60
 H       0.108409     5.322630    -2.027740      24.00
 H       0.098795     5.225940     0.841188      23.62
 H      -1.348371     5.121362    -0.319867      22.06
 C      -1.369176    -0.824520     0.115853      50.98
 H      -1.132922    -1.872835     0.277712      19.77
 C      -3.268408     0.723401    -0.279129      26.75
 H      -4.329236     0.938190    -0.633929      22.69
 C      -2.311651     1.783868     0.271474       0.33
 O      -2.615281     3.133368     0.176790     210.70
 C      -3.606892     3.757728     0.942036     108.97
 H      -3.583125     4.844684     0.977455      25.41
 H      -4.717700     3.174751     0.810929      23.41
 H      -3.512711     3.563733     2.163957      23.95
 C      -0.900978     1.507251     0.294967     -12.70
 O       0.161200     2.531405     0.679174     124.96
 C      -0.378281     0.167353     0.229643      46.27
 H       0.770941    -0.010603     0.133130      19.02
 C      -2.761285    -0.572949    -0.132473      26.04
 C      -3.686875    -1.720141    -0.460189      77.59
 H      -4.431546    -1.664060    -1.295920      20.47
 O      -2.809247    -2.815557    -1.097003     272.40
 H      -3.324840    -3.568789    -1.262831      24.83
 C      -4.249774    -2.276798     0.855601      97.58
 H      -3.374714    -2.530167     1.388052      23.20
 O      -5.014821    -1.175773     1.450154     366.16
 H      -4.877906    -1.115032     2.309386      33.39
 C      -5.286671    -3.664433     0.638922      85.92
 O      -4.961925    -4.885765     0.081508     315.47
 H      -4.256417    -5.246094     0.740334      28.02
 H      -6.142836    -3.052258     0.008232      26.19
 H      -5.904853    -3.896751     1.578280      26.19
55
name = lig-etoh-frame_433
 C       2.410919     1.501226    -2.281303      32.19
 H       1.706363     2.233475    -2.807225      18.12
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 C       3.519473     1.154526    -0.105856      40.50
 H       3.814099     1.256243     0.979811      19.19
 C       4.198656    -0.015599    -0.592532      23.74
 O       4.999847    -0.780455     0.219264     240.62
 C       5.496552    -0.240193     1.505935     108.84
 H       4.584764    -0.088128     2.244777      24.88
 H       6.124833     0.764799     1.553469      26.20
 H       6.000125    -1.037667     1.991504      26.74
 C       3.765865    -0.526075    -1.781813      34.57
 O       3.912471    -1.750876    -2.191381     188.20
 H       4.820767    -2.211572    -1.833035      21.72
 C       2.798144     0.242154    -2.617016      67.20
 H       2.604014    -0.078299    -3.543024      28.88
 C       2.621400     1.928999    -0.937567      70.74
 C       2.027835     3.234657    -0.519879      94.90
 H       2.341126     3.924842    -1.346557      23.80
 O       2.576511     3.754778     0.806057     210.81
 H       3.713877     3.996232     0.831031      23.67
 C       0.442662     3.451033    -0.436610      57.34
 H       0.008853     2.978763    -1.491956      19.41
 C      -0.258826     4.833504    -0.146402     100.74
 O       0.502406     5.733676    -1.128207     300.20
 H       0.167369     5.454282    -1.922519      31.25
 H      -0.032227     5.002552     0.898952      25.86
 H      -1.214810     5.167877    -0.232554      25.23
 C      -1.350553    -0.849991     0.192799      42.58
 H      -1.026180    -2.029877    -0.088411      16.74
 C      -3.206993     0.744155    -0.289373      42.05
 H      -4.175897     0.965765    -0.661771      24.05
 C      -2.319889     1.814879     0.246157      -7.61
 O      -2.604218     3.207836     0.120660     189.73
 C      -3.670636     3.741489     1.019482     122.69
 H      -3.394096     4.822137     1.097041      26.50
 H      -4.644932     3.611999     0.815635      28.56
 H      -3.277162     3.380035     1.869538      27.06
 C      -0.861746     1.536404     0.366337     -16.88
 O       0.098215     2.530268     0.655107     153.88
 C      -0.420753     0.118400     0.176026      37.25
 H       0.641180    -0.032853    -0.041102      20.35
 C      -2.761806    -0.547880    -0.225718      17.45
 C      -3.687769    -1.811935    -0.469373      74.33
 H      -4.420402    -1.642969    -1.280031      21.60
 O      -2.776944    -2.817312    -1.117443     251.56
 H      -3.330231    -3.658162    -1.123260      21.20
 C      -4.277112    -2.281798     0.935952      83.65
 H      -3.377480    -2.468748     1.615598      20.53
 O      -5.031294    -1.176147     1.402403     298.62
 H      -4.642012    -1.215285     2.442223      24.75
 C      -5.316387    -3.606112     0.634446     108.65
 O      -4.988641    -4.958935     0.081733     265.14
 H      -4.130222    -5.379677     0.511520      27.69
 H      -6.293280    -3.421608     0.259355      27.06
 H      -5.860425    -4.011207     1.503726      24.84
55
name = lig-etoh-frame_434
 C       2.359056     1.535973    -2.205127      62.68
 H       1.761734     2.057706    -2.891702      20.41
 C       3.567113     1.209515    -0.185272      64.86
 H       3.541901     1.706474     0.836251      16.17
 C       4.235745    -0.018337    -0.528980      15.76
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 O       5.008505    -0.867380     0.232749     258.27
 C       5.487810    -0.263410     1.483926     114.82
 H       4.638803    -0.232469     2.145121      27.88
 H       5.961356     0.667143     1.465271      29.39
 H       6.121251    -1.121748     1.963122      25.55
 C       3.743932    -0.527994    -1.810176      26.80
 O       3.961451    -1.776418    -2.197582     196.24
 H       4.575599    -2.251343    -1.746570      25.55
 C       2.809970     0.253471    -2.616377      69.11
 H       2.682599    -0.179127    -3.734752      25.59
 C       2.659856     1.880849    -1.000309      50.77
 C       2.041704     3.293864    -0.545612      84.22
 H       2.150012     4.037972    -1.521384      21.06
 O       2.574886     3.781232     0.829476     273.68
 H       3.505822     3.792419     0.663634      28.98
 C       0.453651     3.398658    -0.474790      60.15
 H      -0.138649     2.849921    -1.107654      22.66
 C      -0.203776     4.893835    -0.116518      80.55
 O       0.503283     5.776320    -1.127437     220.29
 H       0.077381     5.748320    -2.262360      18.19
 H       0.041549     5.019902     0.990001      24.34
 H      -1.405608     4.835832    -0.247001      20.87
 C      -1.391038    -0.934315     0.192947      33.17
 H      -1.014568    -1.797887    -0.152484      19.00
 C      -3.116437     0.812586    -0.264510      46.54
 H      -4.135141     1.076274    -0.660724      20.59
 C      -2.281739     1.838821     0.172998      -6.89
 O      -2.615739     3.265568     0.056217     154.38
 C      -3.665376     3.739125     1.093941      86.17
 H      -3.353970     4.779079     1.068183      24.84
 H      -4.848386     3.892774     0.666883      22.73
 H      -3.391073     3.035903     2.004140      22.74
 C      -0.858720     1.530803     0.436177       8.67
 O       0.005764     2.505016     0.636304     165.84
 C      -0.455473     0.161704     0.149262      10.92
 H       0.597663    -0.094525    -0.034613      18.78
 C      -2.732196    -0.583350    -0.293193       2.33
 C      -3.639683    -1.890659    -0.489627      67.50
 H      -4.568390    -1.453524    -1.067165      21.73
 O      -2.764843    -2.832320    -1.122501     237.08
 H      -3.265899    -3.750701    -0.973930      17.84
 C      -4.320932    -2.331541     0.931454      76.85
 H      -3.566281    -2.672097     1.635037      20.95
 O      -5.044685    -1.189164     1.394598     337.44
 H      -4.588912    -1.073784     2.353009      25.11
 C      -5.363953    -3.571655     0.700953      75.19
 O      -4.988832    -5.019013     0.050782     266.13
 H      -4.169559    -5.247748     0.419756      29.24
 H      -6.321866    -3.460972     0.024921      25.81
 H      -5.528509    -3.812877     1.829415      27.09
55
name = lig-etoh-frame_435
 C       2.292318     1.486179    -2.250329      89.63
 H       1.729396     2.037614    -3.054212      22.24
 C       3.631449     1.259344    -0.206112      44.80
 H       3.558116     1.903461     0.647593       9.92
 C       4.205739     0.004920    -0.508361      25.99
 O       5.030062    -0.935615     0.246602     262.89
 C       5.469676    -0.346761     1.483024     121.47
 H       4.555843    -0.233675     2.167292      25.60
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 H       5.926573     0.714554     1.233835      29.00
 H       6.243285    -0.971698     1.801305      27.08
 C       3.695265    -0.472179    -1.811534      25.74
 O       4.006779    -1.843401    -2.243154      71.56
 H       4.639779    -2.356488    -1.431565      20.21
 C       2.865650     0.236753    -2.643078      41.80
 H       2.671116    -0.166166    -3.576078      23.13
 C       2.695038     1.938566    -0.955868      76.70
 C       2.033945     3.367229    -0.556634      91.81
 H       2.249424     4.122753    -1.312606      23.29
 O       2.533497     3.792783     0.802417     264.16
 H       3.611133     3.771218     0.626751      26.13
 C       0.440066     3.344330    -0.452341      39.02
 H      -0.140522     2.915705    -1.419874      21.66
 C      -0.117925     4.906712    -0.151542     104.99
 O       0.487137     5.835078    -1.115832     283.70
 H       0.057556     5.910460    -1.898291      29.97
 H       0.221838     5.316211     0.833408      25.61
 H      -1.070240     4.533485    -0.198144      23.29
 C      -1.447535    -0.933111     0.121929      19.31
 H      -0.853687    -2.047290    -0.151376      15.77
 C      -3.062635     0.846281    -0.249893      38.30
 H      -4.046619     1.172771    -0.576679      20.08
 C      -2.206888     1.882501     0.088524       0.18
 O      -2.657298     3.281136     0.007748     190.42
 C      -3.642381     3.733927     1.123374     107.41
 H      -3.302030     4.756076     1.378536      25.68
 H      -4.529050     3.774391     0.694385      27.96
 H      -3.949430     3.039128     1.927993      25.63
 C      -0.912130     1.481103     0.460067      22.09
 O      -0.051472     2.498664     0.665910     182.66
 C      -0.496937     0.212784     0.169633      20.86
 H       0.622945    -0.081299     0.147642      17.80
 C      -2.690083    -0.645317    -0.300429      18.75
 C      -3.602478    -1.883181    -0.483784      91.24
 H      -4.518596    -1.570734    -0.976792      22.97
 O      -2.785885    -2.877615    -1.113324     290.25
 H      -3.098270    -3.720698    -0.966973      22.28
 C      -4.361787    -2.412483     0.835033      83.92
 H      -3.675117    -2.911609     1.570977      19.19
 O      -5.051567    -1.208363     1.407725     362.77
 H      -4.665925    -0.915870     2.188783      30.64
 C      -5.417169    -3.586471     0.786450      82.70
 O      -4.990718    -5.023796     0.019295     228.26
 H      -4.059976    -5.148547     0.558020      22.28
 H      -6.102684    -3.231776     0.099464      28.74
 H      -5.424436    -3.595081     1.859568      30.30
55
name = lig-etoh-frame_436
 C       2.259322     1.409005    -2.312298      76.35
 H       1.715971     2.045915    -2.983722      24.90
 C       3.690509     1.320862    -0.174188      62.07
 H       4.053269     1.818237     0.855065      18.28
 C       4.143340     0.000661    -0.537274       8.52
 O       5.022829    -0.969640     0.230466     216.87
 C       5.451570    -0.395989     1.473005     123.75
 H       4.670167    -0.245525     2.259996      26.75
 H       5.784654     0.568572     1.163025      29.38
 H       6.415148    -0.917727     1.838154      25.50
 C       3.697630    -0.495656    -1.769352      17.61
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 O       4.056371    -1.892130    -2.262146     206.66
 H       4.563485    -2.167898    -1.496014      24.53
 C       2.903172     0.248261    -2.671833      35.87
 H       2.582771    -0.269375    -3.658228      19.44
 C       2.674914     2.052829    -0.975928      31.60
 C       2.015768     3.382929    -0.520474      90.76
 H       2.480048     4.339380    -1.175418      17.08
 O       2.493233     3.792171     0.742444     269.73
 H       3.513896     4.019612     0.884430      26.45
 C       0.430436     3.313075    -0.431376      70.58
 H       0.237720     3.254404    -1.479569      22.09
 C       0.027165     4.874763    -0.206434      97.18
 O       0.479514     5.903270    -1.051463     205.80
 H      -0.185527     5.891017    -1.992554      22.02
 H       0.340814     5.395223     0.694095      24.25
 H      -1.157111     4.692521    -0.190206      21.67
 C      -1.373596    -0.911691     0.005190      52.87
 H      -1.100766    -1.823416     0.081344      22.28
 C      -3.049757     0.815802    -0.258039      22.71
 H      -4.067318     1.143734    -0.500428      18.64
 C      -2.189827     1.920483     0.012798      -0.06
 O      -2.705954     3.256804    -0.005218     198.86
 C      -3.602368     3.722508     1.118965      93.10
 H      -3.268645     4.561886     1.804570      24.40
 H      -4.624356     3.826350     0.396785      21.84
 H      -4.065839     3.021143     1.882663      24.46
 C      -0.956945     1.473913     0.435732      17.98
 O      -0.057766     2.522498     0.717995     186.82
 C      -0.523152     0.173415     0.235932      49.59
 H       0.494964     0.081465     0.391555      20.94
 C      -2.710852    -0.656265    -0.269992      16.75
 C      -3.610063    -1.856995    -0.454407      90.03
 H      -4.441977    -1.713987    -1.294384      20.48
 O      -2.804950    -2.922368    -1.110309     248.11
 H      -3.155502    -3.866756    -0.918912      17.92
 C      -4.353238    -2.482874     0.755986      98.17
 H      -3.563182    -2.844032     1.469486      20.81
 O      -5.071526    -1.259437     1.391656     261.17
 H      -4.442236    -0.813027     2.265107      21.83
 C      -5.428537    -3.608484     0.811492      80.63
 O      -4.978405    -4.961019     0.031049     252.15
 H      -4.210021    -5.225213     0.602889      27.59
 H      -6.354028    -3.071092     0.281261      26.39
 H      -5.828304    -3.753486     1.897222      27.07
55
name = lig-etoh-frame_437
 C       2.278227     1.397570    -2.286987      67.70
 H       1.661464     2.005342    -2.966353      23.85
 C       3.726378     1.397392    -0.127117      57.59
 H       4.340642     1.564529     0.693877      19.89
 C       4.090618    -0.015486    -0.557411       1.62
 O       4.975989    -0.975893     0.191420     214.42
 C       5.466329    -0.424521     1.460843     119.72
 H       4.753767    -0.395315     2.327940      26.97
 H       5.781434     0.668412     1.274044      27.16
 H       6.311064    -0.934508     1.857256      27.59
 C       3.715593    -0.593796    -1.771791      15.00
 O       4.085599    -1.877248    -2.258312     211.16
 H       4.704577    -2.224246    -1.538292      23.35
 C       2.917974     0.229049    -2.716963      37.58
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 H       2.601360    -0.324899    -3.624742      21.67
 C       2.668493     2.105990    -1.038299      21.50
 C       2.047543     3.387815    -0.484534     111.41
 H       2.285893     4.177397    -1.199298      21.81
 O       2.449712     3.800356     0.743575     300.60
 H       3.353426     4.096956     0.766170      29.62
 C       0.494922     3.374304    -0.410340      69.89
 H       0.227015     3.137560    -1.513486      21.54
 C       0.104599     4.824025    -0.211889     107.73
 O       0.454542     5.979397    -1.036592     260.33
 H       0.117404     5.821851    -1.918889      28.30
 H       0.457400     5.070787     0.867075      25.05
 H      -0.902253     5.157834    -0.122763      24.33
 C      -1.299431    -0.863799    -0.109284      33.08
 H      -1.107435    -2.073988     0.296727      19.03
 C      -3.087169     0.749640    -0.287320      43.55
 H      -4.175548     0.971087    -0.429287      23.59
 C      -2.255350     1.909672    -0.038388      13.38
 O      -2.740185     3.212162     0.007381     220.52
 C      -3.635812     3.691020     1.072993     110.12
 H      -3.234937     4.419350     1.741963      26.90
 H      -4.337639     4.232596     0.552497      27.27
 H      -3.874480     2.746102     1.674779      24.94
 C      -0.959763     1.534678     0.374181       1.36
 O      -0.037067     2.552784     0.753455     148.90
 C      -0.518712     0.131573     0.333088      32.79
 H       0.604720     0.107789     0.700190      21.14
 C      -2.749283    -0.595107    -0.225154       6.72
 C      -3.677167    -1.877125    -0.495092      89.35
 H      -4.247703    -1.637186    -1.337714      22.27
 O      -2.806673    -2.975477    -1.105553     214.10
 H      -3.356650    -3.818952    -0.838134      17.33
 C      -4.324611    -2.502682     0.761054     106.36
 H      -3.427046    -2.684176     1.368100      21.83
 O      -5.072474    -1.318916     1.385594     357.44
 H      -4.398494    -1.138769     1.989508      29.51
 C      -5.461974    -3.624171     0.782546     106.91
 O      -4.988584    -4.844888     0.070056     304.32
 H      -4.311543    -5.296540     0.645049      29.61
 H      -6.406406    -3.318921     0.431260      27.60
 H      -5.958864    -4.014255     1.662728      26.72
55
name = lig-etoh-frame_438
 C       2.334285     1.439007    -2.221711      57.23
 H       1.624044     1.857065    -2.951749      23.41
 C       3.713805     1.393625    -0.176607      71.48
 H       4.449987     1.745814     0.707092      18.38
 C       4.057387    -0.015408    -0.550963      13.62
 O       4.911935    -0.946063     0.160056     207.37
 C       5.479429    -0.419861     1.442799     116.23
 H       4.692027    -0.624623     2.252565      26.24
 H       5.829798     0.633657     1.509203      27.19
 H       6.317146    -1.118674     1.725891      26.63
 C       3.700121    -0.663435    -1.839060      19.18
 O       4.107047    -1.839198    -2.229397     145.12
 H       4.968142    -2.399379    -1.756485      20.61
 C       2.933302     0.164839    -2.714323      50.25
 H       2.635768    -0.285574    -3.667786      22.43
 C       2.728856     2.074446    -1.052653      32.80
 C       2.067446     3.368787    -0.494015      96.77
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 H       2.029240     4.130694    -1.466722      19.34
 O       2.423883     3.816861     0.805302     242.73
 H       3.479804     4.135431     0.560603      22.05
 C       0.564992     3.440553    -0.445507      61.33
 H       0.026103     2.790069    -1.156136      21.97
 C       0.133729     4.840062    -0.131503     100.81
 O       0.473747     6.046697    -1.028783     203.26
 H       0.315242     5.804570    -2.075728      23.30
 H       0.620390     4.812065     0.821389      24.77
 H      -0.943621     5.068962     0.071837      23.98
 C      -1.299318    -0.895264    -0.155464      34.82
 H      -1.014541    -1.801242     0.103385      23.37
 C      -3.191258     0.712630    -0.317749      54.61
 H      -4.249658     0.819883    -0.386867      23.85
 C      -2.335152     1.847921    -0.048060       5.15
 O      -2.757335     3.171361     0.005392     209.16
 C      -3.656974     3.622665     1.024028     103.58
 H      -2.974883     4.340762     1.638502      24.08
 H      -4.431374     4.533956     0.652287      23.31
 H      -3.953081     2.688346     1.461676      25.14
 C      -0.935049     1.602500     0.296029     -11.51
 O      -0.011501     2.583948     0.760664     101.71
 C      -0.452995     0.184971     0.445993       2.53
 H       0.464104    -0.065033     0.862939      22.10
 C      -2.730490    -0.576344    -0.204794      -2.16
 C      -3.710328    -1.915620    -0.567989      59.21
 H      -4.445281    -1.425145    -1.399289      20.62
 O      -2.820961    -3.025705    -1.084634     251.28
 H      -3.387497    -3.727566    -0.906755      22.48
 C      -4.350391    -2.470835     0.799018      85.73
 H      -3.392965    -2.745238     1.382180      19.95
 O      -5.061343    -1.398001     1.371840     363.21
 H      -4.359275    -1.189780     2.120460      25.01
 C      -5.468637    -3.662039     0.738328      81.92
 O      -5.007435    -4.724701     0.091455     291.47
 H      -4.366101    -5.278211     0.734488      26.20
 H      -6.417524    -3.370030     0.108836      25.17
 H      -5.668683    -4.056032     1.815198      25.29
55
name = lig-etoh-frame_439
 C       2.415463     1.435195    -2.200040      50.88
 H       1.651976     1.834746    -2.839835      22.61
 C       3.722442     1.312467    -0.252395      56.82
 H       4.037162     1.982441     0.472448      19.14
 C       4.035502    -0.009787    -0.557070      37.67
 O       4.852989    -0.872014     0.143290     222.78
 C       5.475458    -0.455500     1.439692     122.48
 H       4.685641    -0.692784     2.124521      28.43
 H       5.855235     0.571341     1.568326      27.90
 H       6.281824    -1.215164     1.444829      27.03
 C       3.673177    -0.627162    -1.863697      36.09
 O       4.152365    -1.867415    -2.219726     171.99
 H       4.952585    -2.146689    -1.981093      24.59
 C       2.922916     0.118473    -2.671066      62.32
 H       2.641297    -0.132383    -3.775606      26.93
 C       2.815400     2.027462    -1.001401      62.05
 C       2.052301     3.341764    -0.565576      95.87
 H       2.206182     4.110099    -1.345858      23.86
 O       2.467393     3.848642     0.841052     285.54
 H       3.360716     4.062826     0.851586      29.56
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 C       0.571686     3.428776    -0.489399      58.24
 H       0.002089     2.793840    -1.142392      22.84
 C       0.117813     4.913960    -0.047780      93.44
 O       0.507340     6.085112    -1.013672     179.47
 H       0.448157     5.784605    -2.051628      24.40
 H       0.860359     5.078617     0.832973      22.79
 H      -0.937835     4.627561     0.235682      22.65
 C      -1.316759    -0.833118    -0.114379      28.43
 H      -0.843090    -2.014253    -0.114981      19.73
 C      -3.297438     0.713529    -0.323829      43.20
 H      -4.429367     0.810441    -0.402859      22.60
 C      -2.390568     1.769818    -0.028625      -8.13
 O      -2.767548     3.133649    -0.040327     217.43
 C      -3.650833     3.600038     0.983787     116.97
 H      -2.926296     3.955455     1.674661      25.39
 H      -4.427025     4.236982     0.704488      27.67
 H      -4.371395     2.803189     1.508960      24.67
 C      -0.889843     1.612873     0.253090      -9.03
 O       0.001951     2.620017     0.760112      94.72
 C      -0.456663     0.262032     0.486520      13.68
 H       0.506459    -0.150663     1.000921      21.05
 C      -2.684232    -0.659061    -0.246660       5.23
 C      -3.709193    -1.921907    -0.630537      69.93
 H      -4.511190    -1.591166    -1.212260      23.87
 O      -2.852339    -3.042981    -1.061945     237.23
 H      -3.441168    -3.928758    -1.036174      18.69
 C      -4.394410    -2.446237     0.797943      92.47
 H      -3.612759    -2.901018     1.387216      21.27
 O      -5.031846    -1.451811     1.393134     340.52
 H      -4.719417    -1.018590     2.366127      24.13
 C      -5.478780    -3.629155     0.738137      97.65
 O      -4.987992    -4.700156     0.063200     354.98
 H      -4.384680    -5.093015     0.640995      32.69
 H      -6.227384    -3.245636     0.104285      29.44
 H      -5.518244    -3.662950     1.815867      30.28
55
name = lig-etoh-frame_440
 C       2.491146     1.393405    -2.216869      50.28
 H       1.721014     1.979446    -2.771560      21.77
 C       3.740249     1.244342    -0.291356      75.42
 H       3.849259     1.947196     0.648641      17.22
 C       4.033987    -0.029663    -0.592208      44.25
 O       4.815645    -0.786090     0.138033     241.42
 C       5.455785    -0.522946     1.407413     112.81
 H       4.686651    -0.724130     2.284732      26.57
 H       5.859203     0.561952     1.493500      26.28
 H       6.263224    -1.217488     1.372125      27.15
 C       3.695423    -0.588982    -1.820301      21.19
 O       4.165259    -1.903467    -2.234319     134.44
 H       5.253048    -1.922599    -1.957628      21.49
 C       2.853434     0.154129    -2.669061      61.08
 H       2.683585    -0.081470    -3.642858      29.41
 C       2.833539     1.990525    -0.995233      60.80
 C       2.084609     3.311794    -0.606172      80.63
 H       2.666023     4.206725    -1.169331      21.46
 O       2.504381     3.863874     0.850752     235.05
 H       3.566839     4.049567     1.044246      24.37
 C       0.533914     3.401925    -0.486594      56.26
 H       0.096949     3.165922    -1.571666      22.17
 C       0.134939     4.973351     0.004796      95.37
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 O       0.527989     6.082867    -0.983794     200.89
 H       0.358206     5.833294    -1.844325      30.57
 H       0.712401     5.421754     0.738508      24.74
 H      -0.873804     4.689425     0.269822      23.63
 C      -1.301688    -0.776907    -0.002049      49.98
 H      -0.913337    -1.682028    -0.395359      21.97
 C      -3.348425     0.679207    -0.296801      37.59
 H      -4.379177     0.885141    -0.437636      23.30
 C      -2.411579     1.712521    -0.004365     -19.42
 O      -2.789207     3.082617    -0.113222     199.14
 C      -3.656694     3.534473     0.985935     108.63
 H      -3.089241     3.799018     1.919992      24.90
 H      -4.433470     4.334772     0.479697      23.95
 H      -4.396521     2.921816     1.417463      26.54
 C      -0.865848     1.570250     0.268928     -18.92
 O      -0.001930     2.653759     0.738660     119.43
 C      -0.498449     0.298927     0.466301      61.88
 H       0.447238     0.097630     0.930695      24.09
 C      -2.703704    -0.743307    -0.348941       1.51
 C      -3.655503    -1.936409    -0.601826      78.74
 H      -4.620830    -1.776831    -1.319665      20.47
 O      -2.899955    -3.056438    -1.051946     271.69
 H      -3.414836    -3.899357    -1.155959      21.06
 C      -4.391824    -2.460198     0.752336      99.31
 H      -3.614243    -3.013543     1.423780      20.07
 O      -5.053552    -1.419233     1.464534     370.73
 H      -4.837382    -1.209229     2.277106      32.43
 C      -5.457299    -3.495585     0.737938      84.17
 O      -4.956196    -4.742813     0.006500     270.40
 H      -4.135121    -5.068708     0.577115      27.25
 H      -6.420622    -3.051015     0.259602      27.97
 H      -5.812168    -3.506623     1.842890      28.38
55
name = lig-etoh-frame_441
 C       2.493088     1.420750    -2.255627      56.96
 H       1.903848     2.066950    -2.876399      22.09
 C       3.729764     1.288046    -0.230080      77.05
 H       3.996299     1.333827     0.826072      20.73
 C       4.053823    -0.051409    -0.630562      28.72
 O       4.824853    -0.759887     0.160855     257.05
 C       5.414727    -0.563509     1.381113     130.48
 H       4.882483    -0.727897     2.276047      29.21
 H       5.800591     0.422871     1.421773      27.86
 H       6.313061    -1.272816     1.465497      26.21
 C       3.715541    -0.605284    -1.828085      17.90
 O       4.181634    -1.902164    -2.238978     181.95
 H       5.182007    -1.891765    -1.958341      23.35
 C       2.812872     0.177359    -2.662684      51.02
 H       2.608965    -0.252540    -3.764269      24.31
 C       2.799293     1.958928    -1.033752      53.86
 C       2.202776     3.316248    -0.577121      87.98
 H       2.643696     4.060894    -1.133200      25.73
 O       2.544561     3.857261     0.857679     240.40
 H       3.584884     3.943133     0.829238      26.31
 C       0.517710     3.442634    -0.473684      61.58
 H       0.193661     3.556657    -1.467443      24.52
 C       0.178440     5.012987    -0.001745      80.19
 O       0.536082     6.055492    -0.932773     146.86
 H       0.038954     5.865585    -1.971101      22.44
 H       0.587898     5.463269     1.005723      23.96
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 H      -0.978460     5.182804     0.196228      24.08
 C      -1.352591    -0.751222     0.080706      31.44
 H      -0.723023    -1.676801    -0.380380      19.59
 C      -3.305416     0.593095    -0.252513      29.74
 H      -4.362528     0.946480    -0.491898      17.44
 C      -2.386764     1.684532     0.009001      -7.36
 O      -2.830497     3.016743    -0.165903     180.45
 C      -3.701412     3.496802     0.968168      98.21
 H      -3.291374     3.921293     1.893510      25.87
 H      -3.944159     4.435287     0.467583      25.27
 H      -4.464076     2.591290     1.184714      23.20
 C      -0.933850     1.573663     0.317083      -3.54
 O      -0.027424     2.665774     0.661114     139.41
 C      -0.514873     0.289144     0.430114      44.58
 H       0.548395     0.254983     0.780229      21.63
 C      -2.753969    -0.735008    -0.435962      13.13
 C      -3.641106    -1.978638    -0.551530     105.16
 H      -4.316466    -1.771198    -1.306304      23.67
 O      -2.918043    -3.073392    -1.062712     291.31
 H      -3.550905    -3.773166    -1.155024      22.57
 C      -4.335145    -2.458528     0.754010     106.55
 H      -3.522648    -2.826151     1.310671      24.21
 O      -5.101366    -1.352575     1.510651     235.80
 H      -4.565617    -1.439585     2.546257      21.21
 C      -5.472384    -3.375984     0.709316     101.23
 O      -4.936768    -4.781677    -0.025697     240.60
 H      -4.007613    -4.941668     0.405432      26.11
 H      -6.408131    -3.096541     0.275419      28.05
 H      -5.934361    -3.719471     1.631247      28.21
55
name = lig-etoh-frame_442
 C       2.438880     1.500925    -2.325131      51.92
 H       1.996656     2.131893    -3.127125      19.71
 C       3.699398     1.286507    -0.146568      77.70
 H       4.027805     1.136238     0.892264      20.72
 C       4.078923    -0.003095    -0.641045      12.57
 O       4.857722    -0.823243     0.174249     219.97
 C       5.423364    -0.579982     1.383615     122.52
 H       4.754275    -0.780104     2.360994      25.86
 H       5.885788     0.515468     1.470817      26.30
 H       6.226802    -1.255672     1.473953      27.79
 C       3.700077    -0.645378    -1.909084      17.41
 O       4.184460    -1.869353    -2.240565     197.03
 H       5.052369    -2.094967    -1.956283      25.15
 C       2.830132     0.118515    -2.688628      52.85
 H       2.497442    -0.274626    -3.565238      25.18
 C       2.775917     1.970321    -1.002465      59.47
 C       2.281835     3.333769    -0.477318     101.01
 H       2.463317     4.137161    -1.437062      22.49
 O       2.593373     3.814680     0.830876     292.11
 H       3.587770     3.967689     0.753433      27.90
 C       0.563022     3.578369    -0.417319      51.17
 H       0.005965     3.473412    -1.454277      22.82
 C       0.186441     5.068655     0.014183     117.09
 O       0.543542     6.021347    -0.928212     247.53
 H       0.016157     6.001257    -1.661971      29.59
 H       0.525017     5.119998     1.007921      28.19
 H      -0.831915     5.319021     0.071404      27.21
 C      -1.421281    -0.814523     0.084631      18.43
 H      -0.683299    -1.678455     0.079319      21.44
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 C      -3.229737     0.531041    -0.224148      41.94
 H      -4.215060     0.825448    -0.502326      18.12
 C      -2.340958     1.684213     0.016113      21.88
 O      -2.878058     2.943161    -0.187778     219.82
 C      -3.750680     3.452656     0.911147     107.63
 H      -3.243599     3.807627     1.833143      25.99
 H      -3.972050     4.528032     0.467602      24.74
 H      -4.460656     2.718925     0.936247      25.97
 C      -1.057609     1.623389     0.370185      10.04
 O      -0.078198     2.653947     0.544599     152.00
 C      -0.498498     0.274860     0.406261       1.89
 H       0.633525     0.138149     0.484595      21.15
 C      -2.762042    -0.684831    -0.436895      39.83
 C      -3.638764    -1.994959    -0.521557      82.22
 H      -4.368935    -1.578271    -1.392340      21.83
 O      -2.902196    -3.108622    -1.083520     221.16
 H      -3.765611    -3.772690    -1.150883      16.75
 C      -4.298081    -2.389145     0.790655      89.46
 H      -3.339581    -2.692258     1.421834      21.79
 O      -5.105675    -1.288211     1.586416     276.57
 H      -4.498093    -1.484658     2.345816      25.05
 C      -5.493204    -3.372326     0.651296      85.45
 O      -4.932381    -4.781869    -0.052540     242.48
 H      -4.086275    -4.898454     0.359038      27.60
 H      -6.291438    -3.031032    -0.101141      25.93
 H      -5.725011    -3.918022     1.597062      26.46
55
name = lig-etoh-frame_443
 C       2.409482     1.536643    -2.368562      70.92
 H       2.014860     2.138661    -3.186629      21.48
 C       3.653695     1.198720    -0.101989      48.85
 H       3.813140     1.616311     0.980816      18.39
 C       4.114117     0.038875    -0.644789       8.23
 O       4.880412    -0.925663     0.136851     201.25
 C       5.453155    -0.549451     1.455354     119.06
 H       4.679471    -0.723160     2.138140      27.57
 H       5.858109     0.394651     1.550875      28.75
 H       6.276587    -1.343110     1.511382      25.76
 C       3.702995    -0.636836    -1.933954      13.08
 O       4.163765    -1.845390    -2.269125     124.80
 H       5.045938    -2.389215    -1.774033      19.95
 C       2.843205     0.105901    -2.711038      65.24
 H       2.324098    -0.361238    -3.666367      21.53
 C       2.755936     2.020382    -0.946861      69.31
 C       2.250486     3.396659    -0.439462     102.43
 H       2.376390     4.023710    -1.207724      25.29
 O       2.661887     3.754756     0.791146     282.59
 H       3.697953     4.177723     0.930030      23.99
 C       0.587940     3.698970    -0.402878      52.87
 H       0.180103     3.243894    -1.254611      23.57
 C       0.164537     5.074714     0.041584     111.10
 O       0.607001     6.026818    -0.921934     204.70
 H      -0.083801     6.006070    -1.721971      24.38
 H       0.699027     5.092351     1.054711      25.50
 H      -1.022862     4.998814     0.152355      24.03
 C      -1.393527    -0.870333     0.090023      24.60
 H      -0.971776    -1.933533     0.347247      19.36
 C      -3.168238     0.578003    -0.217819      49.08
 H      -4.240119     0.714472    -0.495765      18.43
 C      -2.382151     1.692531     0.017024      27.77
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 O      -2.932539     2.896717    -0.204219     245.55
 C      -3.764096     3.452436     0.809128     104.83
 H      -3.155817     3.359100     1.769347      24.69
 H      -4.323249     4.402026     0.517998      25.40
 H      -4.812031     2.851158     0.956465      23.71
 C      -1.051952     1.632096     0.410724      12.11
 O      -0.139745     2.641198     0.450485     159.09
 C      -0.532259     0.258531     0.363285      19.67
 H       0.489769     0.001473     0.301086      21.29
 C      -2.708219    -0.739966    -0.360605      32.98
 C      -3.645713    -1.926862    -0.563344      81.52
 H      -4.469575    -1.664333    -1.142560      24.33
 O      -2.911245    -3.150427    -1.100873     267.25
 H      -3.548449    -3.830452    -1.172643      21.43
 C      -4.298940    -2.302164     0.850950      87.98
 H      -3.569745    -2.655863     1.493572      24.05
 O      -5.067363    -1.245934     1.636765     314.65
 H      -4.542557    -1.194403     2.543773      25.30
 C      -5.452798    -3.456985     0.568612      88.05
 O      -4.949051    -4.741085    -0.093224     261.72
 H      -4.076921    -5.012004     0.519027      23.38
 H      -6.044168    -2.991994    -0.205834      27.70
 H      -5.744173    -3.747010     1.580446      28.35
55
name = lig-etoh-frame_444
 C       2.437815     1.511984    -2.325568      40.27
 H       1.925135     2.136045    -3.060414      21.96
 C       3.551129     1.174304    -0.076139      71.20
 H       3.651128     1.841777     0.725494      20.51
 C       4.172387    -0.010467    -0.637651       9.99
 O       4.907753    -1.005307     0.082664     188.52
 C       5.480936    -0.559906     1.495601      86.49
 H       4.511621    -0.663330     2.164294      23.33
 H       5.900327     0.561225     1.561113      23.38
 H       6.217784    -1.315913     1.710017      25.06
 C       3.731995    -0.565990    -1.883379      11.08
 O       4.150400    -1.866961    -2.312878     216.45
 H       4.749941    -2.171443    -1.690328      26.64
 C       2.809136     0.163408    -2.757718      38.03
 H       2.386897    -0.329601    -3.606882      23.12
 C       2.728099     2.040020    -0.956427      67.62
 C       2.143239     3.434457    -0.442906      92.44
 H       2.588116     4.339533    -1.245575      21.35
 O       2.757380     3.722455     0.818689     318.35
 H       3.597798     4.098890     0.789857      32.54
 C       0.611265     3.701167    -0.420659      53.75
 H       0.416415     3.345858    -1.519014      20.62
 C       0.115685     5.038453     0.084690     112.34
 O       0.665495     6.050286    -0.916810     144.75
 H       0.066760     5.924545    -1.846049      23.93
 H       0.701613     5.419701     0.929268      25.79
 H      -0.866289     4.812073     0.313602      25.89
 C      -1.309806    -0.938663     0.108844      58.15
 H      -1.352544    -2.041014     0.443591      17.83
 C      -3.163204     0.605310    -0.250892      45.57
 H      -4.232991     0.729575    -0.452955      22.51
 C      -2.441908     1.700016     0.036633       6.56
 O      -3.006620     2.908828    -0.250325     254.62
 C      -3.831552     3.413519     0.740027     130.62
 H      -3.310636     3.206732     1.651345      26.43
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 H      -4.240588     4.436494     0.509154      26.55
 H      -4.707452     2.934532     0.987504      28.26
 C      -0.968537     1.573536     0.391767      23.40
 O      -0.186093     2.649874     0.421737     159.21
 C      -0.598043     0.231799     0.316911      48.21
 H       0.566158     0.002157     0.311708      20.83
 C      -2.647057    -0.802407    -0.256223      13.18
 C      -3.641655    -1.864728    -0.571935      56.70
 H      -4.657041    -1.701304    -1.164029      21.03
 O      -2.919267    -3.148968    -1.111035     221.51
 H      -3.488881    -3.985270    -1.146626      18.48
 C      -4.346840    -2.241542     0.911784      69.98
 H      -3.594230    -2.785276     1.646230      20.57
 O      -5.002607    -1.225694     1.663995     321.57
 H      -4.691240    -0.780256     2.613195      25.37
 C      -5.346159    -3.533896     0.496784      95.57
 O      -4.947530    -4.686891    -0.114477     313.04
 H      -4.346612    -5.106583     0.473948      31.54
 H      -6.113407    -3.032732    -0.169647      28.04
 H      -6.042492    -3.508293     1.437374      27.94
55
name = lig-etoh-frame_445
 C       2.469628     1.477960    -2.253012      43.77
 H       1.779691     2.106340    -2.851762      22.68
 C       3.423972     1.193182    -0.119138      61.62
 H       3.803302     1.761320     0.870574      19.36
 C       4.204567    -0.076766    -0.600727      15.79
 O       4.960205    -1.045469     0.058043     224.32
 C       5.454122    -0.562624     1.504330     105.52
 H       4.659444    -0.560593     2.162564      28.16
 H       5.831340     0.383999     1.433550      27.78
 H       6.153886    -1.296346     1.897486      26.12
 C       3.737529    -0.496965    -1.870280      -0.18
 O       4.106769    -1.850296    -2.355879     166.57
 H       4.734758    -2.101178    -1.541582      21.19
 C       2.810478     0.249478    -2.735204      40.46
 H       2.468724    -0.248317    -3.687485      22.84
 C       2.693844     2.003183    -1.017497      45.39
 C       2.103500     3.486923    -0.477604      94.19
 H       2.483461     4.210175    -1.003408      24.33
 O       2.801152     3.687847     0.878589     204.74
 H       3.834317     4.043762     0.518798      23.91
 C       0.635719     3.605560    -0.482964      63.35
 H       0.435499     3.793066    -1.551549      21.13
 C       0.134274     5.019738     0.097972      83.33
 O       0.676871     6.054470    -0.925536     158.31
 H       0.437941     5.915838    -1.812143      30.15
 H       0.582277     5.542376     0.938421      23.92
 H      -1.037683     4.968045     0.396485      23.07
 C      -1.303913    -1.040380     0.133830      63.14
 H      -1.024566    -2.050480     0.423189      20.94
 C      -3.190322     0.539219    -0.296520      37.03
 H      -4.235021     0.771538    -0.498235      24.01
 C      -2.427432     1.706992     0.065293     -20.90
 O      -3.074741     2.945195    -0.330665     199.69
 C      -3.925160     3.388981     0.719396     109.07
 H      -3.415053     3.416755     1.765727      24.91
 H      -3.823586     4.566463     0.535545      22.95
 H      -4.889564     2.674824     0.824643      24.10
 C      -0.968310     1.499938     0.292774       1.96
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 O      -0.199342     2.689848     0.436037     132.90
 C      -0.543489     0.184313     0.296336      52.92
 H       0.461713     0.171863     0.471708      23.63
 C      -2.634588    -0.774915    -0.182175      17.06
 C      -3.657761    -1.867357    -0.525811      67.97
 H      -4.373685    -1.549986    -1.241504      23.16
 O      -2.927170    -3.102239    -1.114793     217.35
 H      -3.571383    -3.932651    -0.967398      15.33
 C      -4.355795    -2.263905     0.982563      86.92
 H      -3.584548    -2.726974     1.509144      24.58
 O      -4.974291    -1.189124     1.658605     395.66
 H      -4.476335    -0.962707     2.382318      33.08
 C      -5.319779    -3.475803     0.477528     111.20
 O      -4.934849    -4.662911    -0.140571     275.08
 H      -4.400492    -5.256911     0.487581      29.26
 H      -6.093357    -3.129784    -0.254599      27.07
 H      -6.089574    -3.637849     1.222542      27.10
55
name = lig-etoh-frame_446
 C       2.424834     1.492971    -2.244981      52.58
 H       1.702031     2.046828    -2.795018      22.77
 C       3.394168     1.185967    -0.136260      71.25
 H       3.751454     1.363274     0.786228      21.83
 C       4.151714    -0.083563    -0.570691      15.16
 O       5.027283    -1.050682     0.085081     222.22
 C       5.405056    -0.591371     1.461777     102.88
 H       4.515814    -0.448185     2.240816      24.53
 H       5.938692     0.445758     1.253345      24.84
 H       6.139942    -1.341180     1.936713      25.09
 C       3.727824    -0.487392    -1.911854      13.78
 O       4.050922    -1.779686    -2.368457     123.41
 H       4.784000    -2.271231    -1.697176      20.39
 C       2.872750     0.281465    -2.673537      58.84
 H       2.599414    -0.024273    -3.736135      24.15
 C       2.669528     1.985867    -1.008767      41.36
 C       2.145095     3.438896    -0.457233      79.93
 H       2.488326     4.436150    -1.214030      19.47
 O       2.817753     3.662473     0.900929     291.46
 H       3.723750     3.857972     0.772374      27.64
 C       0.604566     3.546588    -0.505409      67.00
 H       0.203999     3.836398    -1.501125      20.32
 C       0.165119     5.030787     0.072659      90.06
 O       0.664886     6.050858    -0.906237     144.68
 H       0.672389     5.782930    -2.018254      23.13
 H       0.567522     5.332225     1.109026      23.89
 H      -0.858835     5.197530     0.098903      25.79
 C      -1.309493    -1.086346     0.174681      33.13
 H      -0.490752    -1.956468     0.234053      20.01
 C      -3.187089     0.499105    -0.305581      35.32
 H      -4.245931     0.655889    -0.653129      22.81
 C      -2.402576     1.680997     0.035709      -0.44
 O      -3.106708     2.954737    -0.395126     168.72
 C      -4.005891     3.398500     0.734918     122.43
 H      -3.605455     3.411936     1.691290      27.98
 H      -3.997879     4.451163     0.536199      27.08
 H      -4.893538     2.888440     0.560998      27.35
 C      -1.041019     1.481104     0.151767     -10.08
 O      -0.194160     2.720207     0.454997     102.53
 C      -0.447069     0.112644     0.298574      -8.38
 H       0.687348     0.178578     0.685804      19.64
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 C      -2.677494    -0.760240    -0.151404      26.45
 C      -3.630721    -1.902691    -0.433207      72.18
 H      -4.225796    -1.369739    -1.305815      20.95
 O      -2.953360    -3.028676    -1.096498     263.67
 H      -3.537627    -3.700813    -0.854041      20.59
 C      -4.351702    -2.333575     0.960373      80.37
 H      -3.395050    -2.719617     1.529538      20.79
 O      -4.966098    -1.163531     1.624589     336.48
 H      -4.111541    -1.209291     2.396272      20.30
 C      -5.389520    -3.353736     0.491912      87.44
 O      -4.894916    -4.672509    -0.174489     219.30
 H      -4.372222    -5.272076     0.512887      26.61
 H      -5.892834    -2.974139    -0.418830      26.48
 H      -5.966872    -3.873104     1.330549      24.94
55
name = lig-etoh-frame_447
 C       2.332245     1.543048    -2.270391      51.62
 H       1.673242     2.071406    -2.996080      20.88
 C       3.467163     1.091797    -0.138447      52.60
 H       3.588196     1.301035     1.051236      18.04
 C       4.037161    -0.065573    -0.589603      38.24
 O       5.065586    -1.016820     0.127061     210.37
 C       5.365152    -0.593267     1.413639     143.40
 H       4.528892    -0.390642     1.998945      28.49
 H       5.959056     0.270955     1.327038      29.35
 H       5.996767    -1.329259     1.788046      28.26
 C       3.752760    -0.532333    -1.904233      29.04
 O       4.006153    -1.714918    -2.380404     161.36
 H       4.686659    -2.179820    -2.067458      22.97
 C       2.939617     0.298500    -2.661077      56.18
 H       2.741006     0.069687    -3.663901      24.86
 C       2.651306     2.019207    -0.927717      63.15
 C       2.237594     3.374453    -0.452515     105.61
 H       2.418604     4.076300    -1.097576      26.50
 O       2.762287     3.627955     0.903764     291.55
 H       3.847453     3.868858     0.938208      23.18
 C       0.535419     3.562148    -0.456621      59.97
 H       0.097571     3.295072    -1.487897      21.13
 C       0.228687     5.048629     0.011860     106.65
 O       0.670981     6.051852    -0.894665     247.50
 H       0.577580     5.671560    -1.735546      30.98
 H       0.579172     5.022414     1.004601      25.39
 H      -0.924801     5.198134    -0.155239      23.00
 C      -1.231972    -1.031889     0.214913      41.96
 H      -0.695444    -1.881231     0.033591      22.12
 C      -3.173871     0.509216    -0.287424      39.84
 H      -4.136051     0.513000    -0.732824      24.99
 C      -2.437195     1.654620    -0.076341      10.45
 O      -3.103594     2.931084    -0.412074     161.29
 C      -4.054086     3.429138     0.701501      93.56
 H      -3.710440     3.114285     1.788953      24.33
 H      -4.486060     4.558133     0.440282      23.80
 H      -5.142344     3.040551     0.466441      24.45
 C      -1.042826     1.487317     0.041998     -29.68
 O      -0.196779     2.710019     0.460972     119.55
 C      -0.380651     0.082804     0.317784       5.76
 H       0.583189     0.000792     0.652403      21.67
 C      -2.685659    -0.818546    -0.126384      14.88
 C      -3.593949    -1.909702    -0.368126      95.17
 H      -4.346728    -1.477717    -1.021967      23.64
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 O      -2.974629    -2.937566    -1.064560     247.33
 H      -3.544627    -3.855693    -0.829992      13.11
 C      -4.318367    -2.397209     0.872061     107.78
 H      -3.590468    -2.792402     1.542854      22.66
 O      -4.911125    -1.171940     1.603254     345.03
 H      -4.379528    -1.122572     2.453420      27.25
 C      -5.471156    -3.296626     0.515883      74.84
 O      -4.845542    -4.673148    -0.204003     214.30
 H      -4.317523    -5.046262     0.465100      29.51
 H      -5.907740    -2.730974    -0.342856      26.42
 H      -5.936471    -3.761233     1.400606      26.76
55
name = lig-etoh-frame_448
 C       2.278604     1.579191    -2.254261      86.12
 H       1.843008     2.142190    -3.074308      24.68
 C       3.530342     1.050286    -0.077435      68.81
 H       3.451971     1.340026     0.876544      22.19
 C       3.978431    -0.116037    -0.609612      20.96
 O       5.042183    -0.954436     0.109654     199.83
 C       5.355900    -0.575934     1.379024      98.09
 H       4.367028    -0.360251     1.983277      24.99
 H       6.069223     0.369616     1.516302      24.23
 H       5.901997    -1.536799     1.852265      24.19
 C       3.758845    -0.521210    -1.856561      30.43
 O       3.961742    -1.705646    -2.434004     117.59
 H       5.003067    -2.176451    -2.242786      19.27
 C       2.965174     0.363597    -2.677699      37.95
 H       2.857075    -0.063001    -3.799035      20.57
 C       2.647379     1.993911    -0.881985      63.86
 C       2.274121     3.280709    -0.395575      92.25
 H       2.649777     4.130654    -1.303740      20.83
 O       2.699191     3.598179     0.904265     265.56
 H       3.659865     4.009705     0.889894      25.18
 C       0.480815     3.561187    -0.420288      55.58
 H       0.295832     2.979656    -1.325703      21.83
 C       0.226096     5.022453    -0.085247     115.39
 O       0.711658     6.065003    -0.867901     248.26
 H       0.401775     5.691230    -1.833025      24.72
 H       0.624575     5.015632     1.008924      23.74
 H      -0.844160     4.968510     0.057234      24.55
 C      -1.194631    -0.940751     0.219693      49.31
 H      -1.026028    -2.131297     0.005725      18.47
 C      -3.169530     0.463476    -0.268711      30.70
 H      -4.204355     0.538926    -0.734972      21.21
 C      -2.466344     1.669712    -0.219284      -5.07
 O      -3.093828     2.902532    -0.389947     192.27
 C      -4.143130     3.451140     0.629087     110.96
 H      -3.884560     3.041504     1.553160      26.80
 H      -4.332941     4.448320     0.529311      27.87
 H      -5.065081     2.925996     0.507871      27.16
 C      -0.956916     1.502856     0.006366     -28.12
 O      -0.219368     2.660899     0.472029     147.77
 C      -0.398829     0.147368     0.317180      38.81
 H       0.723680    -0.071080     0.551204      21.33
 C      -2.597149    -0.828222    -0.082529      21.46
 C      -3.595460    -1.911930    -0.326615      80.88
 H      -4.647103    -1.538527    -0.833210      20.67
 O      -2.979579    -2.901892    -1.045009     276.59
 H      -3.391406    -3.741617    -0.982993      19.37
 C      -4.294046    -2.418735     0.837299      98.14
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 H      -3.722486    -3.039038     1.623373      20.03
 O      -4.859852    -1.204250     1.565331     319.08
 H      -4.523682    -1.090439     2.563357      25.47
 C      -5.505705    -3.293115     0.514447      76.49
 O      -4.822333    -4.633105    -0.229544     202.54
 H      -4.105646    -4.883742     0.531355      25.50
 H      -6.254108    -2.767833    -0.115189      28.57
 H      -6.128121    -3.491393     1.382807      29.50
55
name = lig-etoh-frame_449
 C       2.310582     1.567550    -2.209984      94.51
 H       1.951270     2.304213    -2.938667      25.47
 C       3.507260     1.098101    -0.056313      55.96
 H       3.598976     1.420358     1.089660      18.36
 C       4.020795    -0.202043    -0.536940      23.12
 O       4.981679    -0.882356     0.030427     218.46
 C       5.358222    -0.554705     1.425337     128.29
 H       4.478658    -0.383587     1.978397      29.79
 H       5.993121     0.270135     1.592891      28.28
 H       5.670842    -1.420382     1.854599      28.64
 C       3.696840    -0.465144    -1.894271      32.66
 O       3.972105    -1.761459    -2.502273     194.15
 H       4.899339    -1.924292    -2.368225      24.55
 C       2.961792     0.430476    -2.717637      33.24
 H       2.909229     0.014623    -3.628242      22.71
 C       2.672503     1.867679    -0.881441      39.80
 C       2.245341     3.267261    -0.366852     105.72
 H       2.678434     3.883419    -0.982891      25.94
 O       2.646443     3.585945     0.920769     303.49
 H       3.482449     4.064094     0.838461      28.10
 C       0.509029     3.486935    -0.423372      68.58
 H       0.433674     3.137498    -1.521379      20.98
 C       0.187636     4.946088    -0.106113     104.50
 O       0.752960     6.051452    -0.883048     185.36
 H       0.324692     6.201451    -1.858157      25.10
 H       0.650384     5.238495     0.800550      25.87
 H      -0.932333     4.967593     0.248515      24.76
 C      -1.235335    -0.942336     0.178811      65.44
 H      -0.996984    -1.943393     0.326999      22.03
 C      -3.179458     0.423249    -0.277908      36.49
 H      -4.208377     0.538781    -0.508838      19.99
 C      -2.426946     1.671050    -0.327277     -19.30
 O      -3.088939     2.896803    -0.362851     184.01
 C      -4.212721     3.390617     0.533418      87.50
 H      -3.861796     3.132929     1.625279      23.93
 H      -3.941566     4.637295     0.572988      21.76
 H      -5.119075     2.778355     0.310807      23.49
 C      -0.897298     1.527037     0.025496      -4.42
 O      -0.247590     2.606776     0.503027     198.59
 C      -0.397290     0.278983     0.299272      50.11
 H       0.681478     0.156968     0.348454      21.69
 C      -2.525835    -0.764916    -0.045999      27.80
 C      -3.626556    -1.898142    -0.313793      78.16
 H      -4.444476    -1.444581    -0.808510      23.32
 O      -2.936927    -2.892915    -1.070646     261.27
 H      -3.502523    -3.737293    -1.062868      16.95
 C      -4.312679    -2.439522     0.931389      86.23
 H      -3.744877    -3.152739     1.549028      21.51
 O      -4.818624    -1.243266     1.510925     317.81
 H      -4.501198    -1.337675     2.607235      21.47
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 C      -5.514556    -3.321184     0.479422      76.44
 O      -4.829971    -4.558106    -0.215051     275.21
 H      -4.047081    -4.793023     0.357938      27.54
 H      -6.419898    -3.002631    -0.119180      27.57
 H      -6.130117    -3.460887     1.492637      28.42
55
name = lig-etoh-frame_450
 C       2.392049     1.550702    -2.179018      64.75
 H       1.933127     2.426766    -2.659653      22.17
 C       3.477824     1.107828    -0.015987      62.06
 H       3.867513     1.447430     0.906830      21.62
 C       4.011996    -0.170401    -0.497549      18.58
 O       4.974248    -0.850541    -0.009286     179.83
 C       5.326227    -0.544144     1.468513      93.72
 H       4.376300    -0.276757     2.068878      25.40
 H       6.079207     0.328210     1.503596      25.41
 H       5.743185    -1.592014     1.888471      24.02
 C       3.623409    -0.449444    -1.957419      30.15
 O       3.981695    -1.788436    -2.564431     164.37
 H       4.974910    -1.910441    -2.399326      23.95
 C       2.954957     0.462079    -2.734004      41.25
 H       2.802466     0.140808    -3.896549      19.79
 C       2.677243     1.777570    -0.858461      38.23
 C       2.136776     3.218876    -0.334836      99.96
 H       2.718379     4.084405    -1.083182      20.65
 O       2.603003     3.578625     0.970664     233.41
 H       3.549915     4.202935     0.873181      22.55
 C       0.608455     3.395029    -0.475214      79.05
 H       0.283093     3.423028    -1.525756      20.62
 C       0.133976     4.885163    -0.082484      89.07
 O       0.772355     6.033721    -0.929400     184.75
 H       0.368570     6.260945    -1.704346      31.01
 H       0.747857     5.273794     0.806105      24.02
 H      -0.911894     5.126712     0.098822      25.39
 C      -1.206951    -0.911912     0.156925      39.37
 H      -0.645096    -1.858960     0.629452      20.05
 C      -3.153938     0.501615    -0.307013      38.54
 H      -4.289411     0.468869    -0.240280      19.25
 C      -2.370048     1.626948    -0.365041       5.52
 O      -3.070394     2.908590    -0.352399     209.41
 C      -4.190990     3.317726     0.476434     120.74
 H      -4.022032     3.187165     1.517774      27.13
 H      -4.054251     4.277433     0.363488      28.50
 H      -5.192068     3.025747     0.025859      25.24
 C      -0.954268     1.562236     0.045708      10.13
 O      -0.240600     2.600811     0.530066     189.74
 C      -0.397623     0.335866     0.251559      30.79
 H       0.705720     0.399539     0.335945      18.98
 C      -2.589103    -0.739896    -0.044489      27.07
 C      -3.586145    -1.886270    -0.291557      51.64
 H      -4.322467    -1.281472    -1.051390      18.88
 O      -2.882306    -2.905871    -1.116330     224.67
 H      -3.686558    -3.594692    -1.176758      15.90
 C      -4.367293    -2.462345     0.988771      74.46
 H      -3.631090    -3.075326     1.596874      20.75
 O      -4.790716    -1.284651     1.506807     417.77
 H      -4.410074    -1.354486     2.339097      28.08
 C      -5.516404    -3.390659     0.472386     102.68
 O      -4.872852    -4.467287    -0.187607     328.56
 H      -4.076216    -4.804652     0.308794      27.79
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 H      -6.190028    -3.129146    -0.335320      27.58
 H      -5.867440    -3.760090     1.414839      27.82
55
name = lig-etoh-frame_451
 C       2.460819     1.585750    -2.147061      27.46
 H       1.856053     2.357850    -2.605386      17.87
 C       3.501536     1.033019     0.032761      72.18
 H       4.006019     1.587850     0.876538      21.53
 C       3.917414    -0.052225    -0.588669      18.19
 O       5.026549    -0.863897     0.024025     186.51
 C       5.291459    -0.560178     1.498206     117.47
 H       4.423819    -0.200542     2.026539      26.23
 H       6.053072     0.209722     1.385459      25.65
 H       5.776526    -1.409599     1.778796      26.37
 C       3.598372    -0.511104    -1.974505      19.31
 O       3.987122    -1.766169    -2.611491     146.73
 H       5.048690    -2.056569    -2.326480      19.57
 C       2.941971     0.426698    -2.826193      44.33
 H       2.727526     0.410653    -3.817155      23.55
 C       2.627476     1.810255    -0.794956      57.03
 C       2.071721     3.182517    -0.347282     118.03
 H       2.306357     3.890477    -0.995456      27.17
 O       2.582156     3.589055     1.026462     318.49
 H       3.360337     4.021347     0.948240      31.44
 C       0.664111     3.374273    -0.509151      75.41
 H       0.079455     3.354922    -1.483972      19.50
 C       0.154725     4.887460    -0.054589      82.72
 O       0.793424     5.996778    -0.947451     150.55
 H       0.180322     5.973672    -1.943732      22.04
 H       0.594791     4.979452     0.935102      25.49
 H      -0.952093     5.061736    -0.128519      23.50
 C      -1.124980    -0.845777     0.168347      36.19
 H      -0.540668    -1.623157     0.649407      19.91
 C      -3.145019     0.575686    -0.332027      42.11
 H      -4.191114     0.619315    -0.121306      21.20
 C      -2.342056     1.648322    -0.332386      30.32
 O      -3.012510     2.912370    -0.364650     229.45
 C      -4.157698     3.228554     0.401133     107.78
 H      -4.251848     2.965188     1.538094      24.65
 H      -4.309220     4.508726     0.097935      22.70
 H      -5.140314     3.152488    -0.087404      24.78
 C      -1.067798     1.596108     0.053893       8.65
 O      -0.203059     2.638622     0.533243     163.08
 C      -0.407177     0.310868     0.180309      18.91
 H       0.684026     0.454362     0.528176      17.03
 C      -2.647869    -0.764697    -0.056278      31.17
 C      -3.523968    -1.884619    -0.305696      83.83
 H      -4.221674    -1.512013    -1.018132      20.40
 O      -2.851014    -2.923338    -1.155665     284.95
 H      -3.554860    -3.467709    -1.336670      23.40
 C      -4.393821    -2.491771     0.928974      82.47
 H      -3.634222    -2.912128     1.638522      19.29
 O      -4.810979    -1.296016     1.537114     373.11
 H      -4.115711    -1.060137     2.506580      18.06
 C      -5.483751    -3.464712     0.504236      79.56
 O      -4.899428    -4.422929    -0.193344     327.06
 H      -4.134209    -4.890857     0.379596      25.35
 H      -6.084828    -2.927682    -0.308787      25.79
 H      -6.020900    -4.102385     1.382513      23.49
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name = lig-etoh-frame_452
 C       2.507183     1.617594    -2.125428      36.47
 H       1.831089     2.203468    -2.792879      19.94
 C       3.487719     1.030504     0.069801      74.30
 H       4.043747     1.565085     0.903129      20.57
 C       3.918994    -0.059939    -0.713774     -14.32
 O       5.042798    -0.870348     0.061274     184.22
 C       5.274071    -0.559698     1.452701      92.24
 H       4.394630    -0.225781     2.077672      24.52
 H       6.050015     0.263340     1.486877      23.38
 H       5.818981    -1.528928     1.918615      23.05
 C       3.590568    -0.581644    -2.011331      18.60
 O       4.015261    -1.723909    -2.629200     237.62
 H       4.720865    -2.098673    -2.264052      29.05
 C       2.926149     0.401083    -2.858261      51.19
 H       2.691121     0.416224    -4.025850      22.30
 C       2.584017     1.886605    -0.713531      47.38
 C       2.062176     3.136818    -0.324607      85.93
 H       2.343389     4.043258    -1.215545      21.48
 O       2.532034     3.585201     1.054139     237.97
 H       3.536127     4.004864     0.916589      24.67
 C       0.562095     3.419082    -0.490488      73.29
 H       0.251646     3.019821    -1.463307      21.16
 C       0.222205     4.908435    -0.061520      95.74
 O       0.779109     5.935199    -0.971096     258.68
 H       0.466242     5.563704    -1.757043      31.29
 H       0.341127     4.873184     1.059910      25.03
 H      -0.891850     4.764102    -0.285821      22.93
 C      -1.119659    -0.796596     0.181688      34.69
 H      -0.601331    -1.746908     0.530832      18.11
 C      -3.155609     0.528787    -0.329868      44.47
 H      -4.236152     0.862231    -0.266540      19.85
 C      -2.385163     1.758182    -0.261702      19.56
 O      -2.933236     2.929888    -0.387907     252.42
 C      -4.165208     3.232000     0.306131     122.50
 H      -4.317866     2.777570     1.277161      26.84
 H      -4.262713     4.190818     0.335623      29.05
 H      -5.082698     2.757255    -0.264307      24.58
 C      -1.046972     1.616061     0.081462      12.96
 O      -0.177737     2.674208     0.514992     192.88
 C      -0.411260     0.346225     0.125832      41.04
 H       0.507509     0.296057     0.601294      19.08
 C      -2.596166    -0.738540    -0.074706      26.50
 C      -3.498791    -1.957470    -0.347626      70.58
 H      -4.441517    -1.598029    -1.019606      19.24
 O      -2.801488    -2.928408    -1.180649     241.78
 H      -3.535976    -3.603149    -1.529743      19.88
 C      -4.350509    -2.484768     0.877595     107.60
 H      -3.692956    -3.023893     1.563094      20.39
 O      -4.845534    -1.267293     1.617393     421.51
 H      -4.239658    -1.140375     2.206896      33.57
 C      -5.492311    -3.486319     0.578029     103.03
 O      -4.871409    -4.475559    -0.256766     359.49
 H      -4.278415    -4.897856     0.316235      33.83
 H      -6.193970    -2.787953     0.096852      28.54
 H      -6.210962    -3.844818     1.265140      27.92
55
name = lig-etoh-frame_453
 C       2.520450     1.598970    -2.142439      51.35
 H       1.949130     2.196169    -2.847542      21.63
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 C       3.436776     1.072134     0.028781      62.15
 H       3.954717     1.309212     0.941662      20.74
 C       4.010566    -0.137318    -0.750872      -1.23
 O       5.016934    -0.874254     0.060575     236.33
 C       5.293197    -0.562388     1.407334     116.14
 H       4.380167    -0.395390     2.030008      25.81
 H       5.934710     0.313929     1.666840      25.65
 H       5.607462    -1.414793     1.936631      26.11
 C       3.578072    -0.588862    -2.073773      12.88
 O       4.035881    -1.688568    -2.654047     166.47
 H       4.708133    -2.286988    -1.960354      21.37
 C       2.902814     0.416728    -2.823304      56.43
 H       2.777846     0.193808    -3.871568      21.38
 C       2.600329     1.894056    -0.686017      29.01
 C       2.061539     3.218867    -0.295866     111.71
 H       2.541646     3.808315    -0.924383      25.14
 O       2.496250     3.592283     1.037377     281.01
 H       3.524496     3.850754     0.929841      25.67
 C       0.462064     3.457564    -0.437069      77.26
 H       0.454711     2.940387    -1.445215      19.48
 C       0.250495     4.885701    -0.112185     114.57
 O       0.771840     5.857719    -0.945011     294.39
 H       0.697163     5.418866    -1.941461      25.15
 H       0.218480     5.116263     0.985789      24.20
 H      -0.838410     4.787279    -0.262108      22.81
 C      -1.201866    -0.805161     0.180273      47.00
 H      -0.805084    -1.892192     0.226415      17.20
 C      -3.167255     0.513502    -0.302867      48.03
 H      -4.211491     0.670933    -0.640844      17.93
 C      -2.415060     1.773753    -0.163724      -3.08
 O      -2.874731     3.016140    -0.411356     215.48
 C      -4.213078     3.175825     0.183125      91.36
 H      -4.159039     2.598611     1.174874      24.34
 H      -4.239531     4.424797     0.610805      21.61
 H      -4.853527     2.586333    -0.420614      24.14
 C      -0.952078     1.653005     0.111438      17.74
 O      -0.183599     2.696236     0.502694     238.73
 C      -0.408904     0.412781     0.115176      35.82
 H       0.658140     0.206068     0.600504      16.53
 C      -2.516852    -0.714429    -0.112787      14.46
 C      -3.537090    -2.028641    -0.419192      70.92
 H      -4.375747    -1.578784    -0.925754      21.43
 O      -2.749229    -2.941530    -1.202457     268.58
 H      -3.387732    -3.665420    -1.525133      19.71
 C      -4.279730    -2.466915     0.899863      91.29
 H      -3.616834    -3.153595     1.535677      19.26
 O      -4.909818    -1.262631     1.647953     297.23
 H      -4.019799    -1.210885     2.474385      17.67
 C      -5.501981    -3.436067     0.614566      67.60
 O      -4.865733    -4.548530    -0.338626     257.04
 H      -4.193034    -5.049119     0.303146      26.66
 H      -6.338076    -2.828922     0.112406      27.84
 H      -6.197267    -3.686918     1.607798      26.91
55
name = lig-etoh-frame_454
 C       2.495400     1.575271    -2.166044      51.92
 H       2.060196     2.402408    -2.754629      20.29
 C       3.434622     1.039746    -0.076487      67.00
 H       3.675247     1.040331     1.080915      17.08
 C       4.094904    -0.175449    -0.701689      19.66
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 O       4.978410    -0.889109     0.010274     229.38
 C       5.276233    -0.552469     1.401199     105.25
 H       4.278884    -0.453954     1.887945      25.00
 H       5.849131     0.360318     1.545988      26.77
 H       5.694502    -1.544531     1.860639      23.91
 C       3.601519    -0.536136    -2.058133      28.65
 O       4.083834    -1.705605    -2.683470     202.08
 H       4.500508    -2.196392    -1.907799      26.14
 C       2.891091     0.423695    -2.743644      53.47
 H       2.748890     0.109084    -3.808844      19.90
 C       2.622034     1.876770    -0.751537      26.45
 C       2.055301     3.300795    -0.232598     100.58
 H       2.759496     4.039147    -0.977275      19.19
 O       2.481773     3.607916     1.016195     317.57
 H       3.382577     3.779484     1.010601      29.87
 C       0.505574     3.455920    -0.404439      94.13
 H       0.246898     3.272618    -1.464236      20.06
 C       0.159820     4.865560    -0.160308     112.54
 O       0.799579     5.785883    -0.935898     282.93
 H       0.776868     5.741980    -1.948214      28.53
 H       0.443642     5.302692     0.826629      24.07
 H      -0.973954     5.118486    -0.200449      23.33
 C      -1.241254    -0.820006     0.145344      46.66
 H      -0.871341    -1.796409     0.044607      17.43
 C      -3.161312     0.573755    -0.284590      53.23
 H      -4.089635     0.324997    -0.871318      14.26
 C      -2.381114     1.708974    -0.072237     -10.83
 O      -2.835226     3.125308    -0.424314     196.55
 C      -4.226121     3.148652     0.122994     104.83
 H      -4.084947     2.505374     0.989321      26.34
 H      -4.459307     4.040701     0.391048      28.29
 H      -4.973241     2.743337    -0.713772      25.15
 C      -0.928752     1.680483     0.130800      15.92
 O      -0.208928     2.721558     0.528075     253.76
 C      -0.370254     0.382232     0.174874      32.27
 H       0.645305     0.352154     0.312192      16.82
 C      -2.551168    -0.736905    -0.178633      28.52
 C      -3.543032    -2.024874    -0.454333      50.45
 H      -4.367454    -1.523626    -1.159368      20.78
 O      -2.704977    -2.965822    -1.218818     279.59
 H      -3.255274    -3.700556    -1.381137      21.27
 C      -4.243247    -2.478628     0.947852      77.16
 H      -3.521446    -2.981189     1.554489      19.58
 O      -4.903962    -1.292060     1.682339     349.33
 H      -4.463574    -1.256362     2.520514      27.48
 C      -5.501765    -3.366834     0.636872      82.65
 O      -4.892117    -4.609611    -0.381493     232.77
 H      -4.179441    -5.076423     0.160856      26.42
 H      -6.214298    -3.071023    -0.111918      29.00
 H      -5.680326    -3.745564     1.621417      29.87
55
name = lig-etoh-frame_455
 C       2.430676     1.625549    -2.167272      21.41
 H       2.114282     2.508194    -2.740168      17.31
 C       3.484767     0.924871    -0.136689      85.19
 H       3.320316     1.045320     0.880586      18.06
 C       4.097096    -0.134686    -0.671016      28.25
 O       4.969095    -0.934752    -0.043607     233.40
 C       5.227410    -0.578148     1.402628     103.69
 H       4.223414    -0.445844     1.882916      25.63
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 H       5.803302     0.394061     1.305074      26.76
 H       5.911245    -1.403891     1.638642      24.40
 C       3.693649    -0.500560    -1.966880      37.50
 O       4.117518    -1.714414    -2.701920     217.94
 H       4.516621    -2.208840    -2.009113      29.25
 C       2.887423     0.392022    -2.703823      54.83
 H       2.596710     0.204380    -3.805065      20.18
 C       2.623385     1.892236    -0.865004      82.95
 C       2.100626     3.343010    -0.267843     111.67
 H       2.344442     4.107571    -0.908368      19.27
 O       2.465227     3.633248     1.037771     264.88
 H       3.602134     3.835142     1.095692      23.99
 C       0.592652     3.475689    -0.416250      88.58
 H       0.059280     3.446674    -1.398468      16.26
 C       0.006765     4.913506    -0.154889     111.38
 O       0.879240     5.777319    -0.963446     235.52
 H       0.549367     5.789900    -1.886199      29.51
 H       0.637705     5.150281     0.764854      22.86
 H      -1.007727     5.149476    -0.148382      25.52
 C      -1.208126    -0.810962     0.087469      33.92
 H      -0.638272    -1.871572    -0.030352      15.35
 C      -3.143940     0.590550    -0.290147      56.98
 H      -4.068054     0.499745    -0.926279      16.67
 C      -2.323864     1.713862    -0.033635     -11.72
 O      -2.807938     3.182953    -0.411334     171.60
 C      -4.223886     3.082732     0.026840      99.56
 H      -4.372577     2.401654     0.903998      25.82
 H      -4.778266     4.285855     0.285003      22.79
 H      -4.960303     2.955659    -0.707508      26.03
 C      -0.969119     1.618588     0.163004      17.53
 O      -0.234424     2.752614     0.583185     208.76
 C      -0.370591     0.315123     0.248218      25.62
 H       0.807021     0.363674     0.081091      16.04
 C      -2.661313    -0.754015    -0.238822      39.67
 C      -3.514789    -1.939918    -0.475293      62.40
 H      -4.249065    -1.744361    -1.277340      18.93
 O      -2.674533    -2.984535    -1.214115     213.63
 H      -3.269439    -3.896214    -1.159961      14.71
 C      -4.252799    -2.457972     0.946631      78.08
 H      -3.412785    -2.848581     1.629861      15.69
 O      -4.897034    -1.346525     1.675324     305.11
 H      -4.551408    -1.307119     2.711774      22.67
 C      -5.410554    -3.350108     0.624802      85.82
 O      -4.933126    -4.648058    -0.394267     244.04
 H      -4.215675    -5.043887     0.091432      26.97
 H      -6.205810    -3.143441    -0.127712      27.01
 H      -5.496189    -4.032214     1.595210      26.59
55
name = lig-etoh-frame_456
 C       2.370736     1.684673    -2.216261      62.16
 H       1.989017     2.407163    -2.930068      19.00
 C       3.452429     0.923401    -0.153875      62.72
 H       3.205606     1.135354     0.953406      17.24
 C       4.100858    -0.125498    -0.683735      35.02
 O       4.980053    -1.004395    -0.068052     254.95
 C       5.195379    -0.595455     1.344490     112.10
 H       4.344282    -0.534747     2.036635      26.71
 H       5.667004     0.365845     1.287416      27.50
 H       5.994202    -1.292711     1.681229      25.12
 C       3.778662    -0.494684    -1.963443      29.99
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 O       4.132028    -1.682276    -2.690273     147.25
 H       4.826237    -2.407009    -2.112473      18.47
 C       2.875511     0.367235    -2.694751      70.17
 H       2.580017     0.189927    -3.679636      23.34
 C       2.658707     1.923993    -0.906018      90.08
 C       2.128435     3.318389    -0.347673      95.24
 H       2.275058     4.320921    -1.102927      17.68
 O       2.501767     3.670119     1.073257     320.95
 H       3.379672     3.912336     1.042162      30.69
 C       0.573911     3.521275    -0.428496      68.64
 H       0.228379     3.141772    -1.440349      16.82
 C      -0.008756     4.982279    -0.098607      92.29
 O       0.952086     5.806764    -1.015026     204.77
 H       0.247004     5.715535    -1.848552      23.43
 H       0.285329     5.024611     0.940427      25.86
 H      -1.198373     5.026987    -0.147375      22.09
 C      -1.169940    -0.842287     0.002443      43.50
 H      -0.652630    -1.687562    -0.019331      18.40
 C      -3.138693     0.576138    -0.331719      34.21
 H      -4.112187     0.998530    -0.747331      16.57
 C      -2.304121     1.780036    -0.055604     -13.57
 O      -2.806471     3.166989    -0.361005     216.64
 C      -4.254045     3.110907    -0.048063     117.89
 H      -4.699904     2.438225     0.728824      26.47
 H      -4.505378     3.990877     0.232140      28.40
 H      -4.918882     2.826441    -1.016585      25.01
 C      -0.971252     1.548408     0.243109      18.91
 O      -0.256911     2.759634     0.633007     180.42
 C      -0.378158     0.262011     0.293113      39.79
 H       0.645282     0.156799     0.087630      18.82
 C      -2.677464    -0.718013    -0.259662      27.05
 C      -3.484137    -1.889087    -0.501916      69.62
 H      -4.339030    -1.778765    -1.255243      17.51
 O      -2.668684    -3.015236    -1.172169     249.31
 H      -3.195789    -3.780737    -0.959762      15.75
 C      -4.240912    -2.391376     0.911858      92.44
 H      -3.486538    -2.886027     1.465969      19.05
 O      -4.904091    -1.398262     1.647495     341.77
 H      -4.359366    -1.465959     2.641535      19.17
 C      -5.282986    -3.458598     0.592985     109.46
 O      -4.973751    -4.655480    -0.392072     313.16
 H      -4.173582    -5.103030     0.164653      27.66
 H      -6.221635    -2.946508     0.244909      28.00
 H      -5.732673    -4.005786     1.362708      28.24
55
name = lig-etoh-frame_457
 C       2.359568     1.665249    -2.306297      52.02
 H       1.757227     2.220956    -3.072190      19.36
 C       3.343499     1.043229    -0.113285      36.38
 H       3.495669     1.132449     0.929140      17.94
 C       4.133000    -0.168054    -0.705436      18.94
 O       4.981676    -1.068623    -0.055780     265.12
 C       5.205580    -0.616249     1.267995     119.45
 H       4.411156    -0.756973     2.093000      24.85
 H       5.513196     0.482711     1.366667      26.34
 H       5.998434    -1.245037     1.823140      25.15
 C       3.810092    -0.493531    -2.068834      17.30
 O       4.162816    -1.658092    -2.651833     215.66
 H       4.929550    -2.065734    -2.387696      25.61
 C       2.863065     0.382648    -2.682220      45.20
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 H       2.608460    -0.057866    -3.784817      23.02
 C       2.702279     1.984274    -0.900769      35.13
 C       2.127283     3.319690    -0.409536      91.14
 H       2.542154     4.049167    -1.017382      21.93
 O       2.527201     3.699141     1.056606     253.74
 H       3.586267     4.093730     1.008294      22.76
 C       0.489096     3.530542    -0.421611      48.85
 H       0.404300     2.967627    -1.367995      17.01
 C       0.053843     5.005533    -0.045803      95.79
 O       0.951589     5.849100    -1.051205     223.94
 H       0.490851     5.744144    -1.878031      28.40
 H      -0.081397     5.189991     1.099473      24.60
 H      -0.943812     4.987065    -0.353707      24.45
 C      -1.201633    -0.857288    -0.081487      43.09
 H      -0.676619    -1.956289    -0.079606      15.71
 C      -3.135514     0.645707    -0.388690      50.79
 H      -4.173239     1.071364    -0.404945      16.15
 C      -2.309645     1.814441    -0.109677      -6.77
 O      -2.820070     3.082018    -0.274626     211.15
 C      -4.308793     3.122989    -0.169674      88.74
 H      -4.682373     2.443826     0.595321      26.56
 H      -4.396945     4.366625     0.293108      21.52
 H      -4.633233     2.831111    -1.110759      25.18
 C      -0.941015     1.555908     0.348069       5.90
 O      -0.264433     2.739365     0.667720     196.61
 C      -0.410581     0.221478     0.305912      35.30
 H       0.719713    -0.001130     0.323225      15.67
 C      -2.586618    -0.661543    -0.272864      31.99
 C      -3.493635    -1.902620    -0.536187      71.49
 H      -4.424404    -1.589591    -1.146454      18.71
 O      -2.675310    -3.020435    -1.093521     261.86
 H      -3.216177    -3.804590    -0.879828      15.32
 C      -4.195548    -2.367276     0.833036      99.50
 H      -3.354741    -2.925626     1.391314      16.51
 O      -4.904104    -1.442035     1.628264     384.66
 H      -4.233750    -1.427415     2.413313      22.52
 C      -5.217678    -3.598334     0.527497      99.99
 O      -4.988494    -4.636102    -0.364924     371.81
 H      -4.360451    -5.182184     0.104896      34.40
 H      -6.034827    -2.813442     0.396825      26.08
 H      -5.839655    -3.942241     1.513622      27.18
55
name = lig-etoh-frame_458
 C       2.390276     1.591731    -2.358170      50.73
 H       1.631420     2.058307    -2.952249      19.97
 C       3.311251     1.101812    -0.081934      54.11
 H       3.751710     1.316299     0.928343      18.63
 C       4.108120    -0.166259    -0.749929       8.01
 O       4.966476    -1.110695    -0.035414     244.47
 C       5.247805    -0.633438     1.270182     120.19
 H       4.353375    -0.903334     1.824964      25.72
 H       5.369897     0.424291     1.339827      27.41
 H       6.043247    -1.207451     1.639795      26.16
 C       3.817319    -0.447907    -2.113763       9.12
 O       4.186363    -1.645003    -2.649156     162.65
 H       5.247594    -1.804365    -2.403213      22.46
 C       2.852036     0.379643    -2.751831      39.44
 H       2.626269    -0.065746    -3.618972      24.83
 C       2.693871     2.054265    -0.934678      19.93
 C       2.115345     3.325708    -0.373206      87.51
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 H       2.767947     4.061405    -1.109562      16.46
 O       2.567618     3.728220     0.989480     309.57
 H       3.529025     4.072442     1.003266      25.99
 C       0.449988     3.501178    -0.360147      47.89
 H       0.104744     3.123186    -1.412364      16.96
 C       0.135021     4.991069    -0.068407     107.69
 O       0.929728     5.898527    -1.024933     218.25
 H       0.628811     5.713977    -2.025736      25.86
 H       0.025658     5.435985     0.888392      26.19
 H      -0.850127     5.124923    -0.680076      21.09
 C      -1.227814    -0.895433    -0.143464      51.11
 H      -0.982486    -1.882207    -0.191543      16.81
 C      -3.112213     0.745406    -0.410819      69.31
 H      -4.232197     0.616364    -0.312933      18.15
 C      -2.295346     1.774058    -0.151374      12.29
 O      -2.835907     2.994741    -0.169929     203.01
 C      -4.324107     3.199680    -0.255759      98.38
 H      -4.673475     2.481972     0.533594      24.90
 H      -4.476579     4.157547    -0.055133      27.28
 H      -4.628026     3.018197    -1.382990      24.05
 C      -0.934047     1.591143     0.413755      -1.35
 O      -0.240479     2.716999     0.700549     228.81
 C      -0.412472     0.210740     0.298652      30.18
 H       0.596069     0.041086     0.775388      14.96
 C      -2.528678    -0.627417    -0.322866      19.75
 C      -3.515978    -1.897781    -0.542034      71.58
 H      -4.323625    -1.501922    -1.231276      18.63
 O      -2.699279    -3.003663    -1.002426     250.32
 H      -3.270284    -3.918364    -0.935312      13.36
 C      -4.104940    -2.445923     0.747440     107.75
 H      -3.245707    -2.703655     1.351629      18.05
 O      -4.896736    -1.487890     1.601636     357.19
 H      -4.098792    -1.122655     2.362303      20.30
 C      -5.232687    -3.639661     0.542450      92.79
 O      -4.993050    -4.628895    -0.358043     377.00
 H      -4.470709    -5.351717     0.075650      32.26
 H      -5.975522    -3.025725    -0.033048      28.10
 H      -5.403637    -3.922521     1.534135      27.56
55
name = lig-etoh-frame_459
 C       2.413260     1.552608    -2.326785      40.97
 H       1.552372     2.045277    -2.838567      17.74
 C       3.377720     1.097123    -0.097998      76.34
 H       3.736777     1.618614     0.812268      20.42
 C       4.042714    -0.112602    -0.763532      11.69
 O       4.928545    -1.112843    -0.060147     223.56
 C       5.268473    -0.661618     1.298917      86.73
 H       4.306268    -0.947862     1.832730      22.27
 H       5.405253     0.459175     1.316850      23.32
 H       6.299715    -1.231426     1.489374      23.22
 C       3.809213    -0.386902    -2.083224       8.48
 O       4.239706    -1.650988    -2.667275     173.40
 H       5.282786    -1.612981    -2.416920      21.70
 C       2.877833     0.342463    -2.844438      27.30
 H       2.412268    -0.078351    -3.895420      22.01
 C       2.659597     2.048362    -0.983465      56.45
 C       2.124362     3.365535    -0.331933     100.24
 H       2.381054     4.123430    -1.066953      18.81
 O       2.574461     3.740027     0.912713     312.37
 H       3.665289     4.007955     0.875583      24.74
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 C       0.464814     3.466566    -0.297687      61.72
 H      -0.160193     3.404985    -1.208841      17.05
 C       0.172637     4.996679    -0.208754     109.78
 O       0.918961     5.945002    -0.978936     239.36
 H       0.642011     5.623492    -1.908372      28.74
 H       0.337527     5.539830     0.781036      24.48
 H      -0.838313     5.182661    -0.541354      25.12
 C      -1.210824    -0.885131    -0.170824      32.94
 H      -0.984039    -2.042897    -0.236678      13.57
 C      -3.105735     0.692246    -0.417173      62.77
 H      -4.173199     0.380761    -0.406220      15.20
 C      -2.267576     1.742194    -0.147726      18.76
 O      -2.855252     2.978344    -0.064501     202.37
 C      -4.292230     3.211577    -0.366858      93.37
 H      -4.925507     2.638658     0.318992      25.14
 H      -4.600883     4.500194    -0.191153      22.89
 H      -4.687167     3.126879    -1.331377      26.15
 C      -0.953402     1.562028     0.400892      -0.03
 O      -0.186149     2.710420     0.748426     247.18
 C      -0.408658     0.241190     0.319729      41.96
 H       0.442283     0.104683     0.978310      15.59
 C      -2.571779    -0.598175    -0.412780      22.98
 C      -3.521297    -1.854054    -0.535305      83.56
 H      -4.190989    -1.606115    -1.461271      17.57
 O      -2.722547    -3.000170    -0.935730     283.63
 H      -3.272283    -3.734756    -1.007392      19.67
 C      -4.049535    -2.522465     0.707460     100.87
 H      -3.139420    -2.705191     1.325697      16.51
 O      -4.858434    -1.520666     1.564069     433.96
 H      -4.364394    -1.167095     2.178664      32.83
 C      -5.235091    -3.567010     0.565368      82.94
 O      -4.974253    -4.678964    -0.386513     301.83
 H      -4.522664    -5.502569     0.078119      29.71
 H      -6.089411    -3.285050    -0.094892      25.16
 H      -5.189335    -3.998097     1.665817      23.94
55
name = lig-etoh-frame_460
 C       2.386626     1.549129    -2.273869      60.08
 H       1.638604     2.102069    -2.826336      18.10
 C       3.481337     1.107662    -0.183713      51.59
 H       3.674491     1.609673     0.749389      14.46
 C       3.991030    -0.036424    -0.691237      31.31
 O       4.866619    -1.064245    -0.114095     236.30
 C       5.286744    -0.696445     1.304350     135.49
 H       4.605725    -0.923684     2.135127      27.16
 H       5.519169     0.358987     1.369843      27.85
 H       6.174844    -1.147924     1.490171      27.80
 C       3.778329    -0.391925    -2.099300      43.77
 O       4.308636    -1.621624    -2.675185     223.70
 H       5.162251    -1.796105    -2.433738      23.84
 C       2.894587     0.312241    -2.949494      21.37
 H       2.465515     0.061109    -3.821076      22.14
 C       2.650308     1.962262    -0.994219      60.44
 C       2.070668     3.374420    -0.365954      94.63
 H       2.076483     4.326833    -1.150916      17.83
 O       2.587934     3.752511     0.862939     311.79
 H       3.611469     3.841029     0.766299      26.19
 C       0.511664     3.460750    -0.257436      75.20
 H      -0.140606     3.240914    -1.200165      17.04
 C       0.177414     5.054345    -0.267336     109.72
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 O       0.922771     5.969590    -0.974537     249.34
 H       0.712086     5.795668    -1.885118      31.38
 H       0.506838     5.249888     0.771290      25.97
 H      -1.003750     5.125723    -0.264459      24.25
 C      -1.181646    -0.847400    -0.171804      45.40
 H      -0.765153    -1.860669    -0.136436      17.13
 C      -3.123618     0.556208    -0.425345      23.63
 H      -4.233532     0.783547    -0.548522      14.31
 C      -2.282782     1.738983    -0.106379       9.54
 O      -2.886121     3.016894     0.030565     204.64
 C      -4.265967     3.265534    -0.441325     120.86
 H      -5.150402     2.817123     0.104237      25.66
 H      -4.355400     4.258340    -0.269102      26.63
 H      -4.558954     2.999024    -1.561353      25.24
 C      -0.965171     1.531314     0.332582       9.05
 O      -0.132136     2.696558     0.815952     208.78
 C      -0.427618     0.253926     0.352030      48.89
 H       0.533034     0.079478     1.009628      14.75
 C      -2.597236    -0.641108    -0.503186      35.15
 C      -3.502983    -1.816572    -0.573789     106.20
 H      -4.226536    -1.737765    -1.400293      19.82
 O      -2.705495    -2.996037    -0.910163     257.75
 H      -3.449561    -3.734968    -1.060725      14.07
 C      -4.066693    -2.510310     0.729949      85.14
 H      -3.192802    -3.014352     1.228426      17.26
 O      -4.841380    -1.566055     1.478831     346.66
 H      -4.242989    -1.200811     2.446037      18.52
 C      -5.183971    -3.526554     0.577859     110.13
 O      -4.939990    -4.758196    -0.422958     323.01
 H      -4.505407    -5.403092     0.096088      34.90
 H      -6.264448    -3.154917     0.420060      28.16
 H      -5.411694    -3.949697     1.507483      28.45
55
name = lig-etoh-frame_461
 C       2.333978     1.520539    -2.281744      47.78
 H       1.747943     2.225095    -2.900405      20.52
 C       3.568632     1.184754    -0.249898      85.26
 H       3.713398     1.350860     0.877845      13.80
 C       3.987512    -0.040784    -0.670555      37.54
 O       4.792162    -0.976533    -0.129197     235.78
 C       5.294421    -0.714951     1.284747     122.07
 H       4.805782    -0.963272     2.292092      27.02
 H       5.593459     0.356948     1.380363      28.87
 H       6.305013    -1.356125     1.464261      26.05
 C       3.746822    -0.448834    -2.148892      13.01
 O       4.352173    -1.559675    -2.682659     115.95
 H       5.243314    -2.149331    -2.184406      17.59
 C       2.910368     0.353345    -2.948660      49.27
 H       2.562229     0.037346    -4.059438      20.72
 C       2.644928     1.900324    -0.976066      50.86
 C       1.979555     3.349383    -0.470490      94.25
 H       2.193653     4.148077    -1.199328      19.95
 O       2.579010     3.752562     0.827783     250.83
 H       3.677677     3.888002     0.827621      25.52
 C       0.527939     3.459253    -0.282338      73.34
 H       0.268193     2.873601    -1.196579      18.07
 C       0.145229     5.072822    -0.189078     106.88
 O       0.930561     5.992043    -1.008099     200.60
 H       0.733674     6.071310    -2.051824      25.53
 H       0.484463     5.113256     0.859525      26.09
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 H      -0.937900     5.142745    -0.099912      25.27
 C      -1.163588    -0.786645    -0.150837      49.96
 H      -0.608521    -1.716678    -0.053879      16.99
 C      -3.169293     0.555538    -0.425424      40.69
 H      -4.069260     1.116155    -0.719797      13.19
 C      -2.357232     1.722019    -0.051076      -1.32
 O      -2.921821     3.046919     0.114208     193.38
 C      -4.246379     3.277979    -0.535203      92.78
 H      -5.087788     2.882933     0.019808      26.19
 H      -4.195974     4.591749    -0.356803      21.84
 H      -4.099552     2.943461    -1.543692      25.89
 C      -0.953757     1.571676     0.271284       4.43
 O      -0.095857     2.664647     0.880827     173.18
 C      -0.439354     0.229418     0.389336      34.17
 H       0.517523     0.078141     0.728528      17.06
 C      -2.554415    -0.761851    -0.565621      27.01
 C      -3.474222    -1.860944    -0.625660      88.50
 H      -4.486113    -1.733153    -1.251279      20.43
 O      -2.671839    -3.017371    -0.934033     258.54
 H      -3.406599    -3.726332    -1.086608      13.72
 C      -4.109683    -2.454070     0.760235      89.62
 H      -3.346782    -3.103362     1.191276      16.74
 O      -4.809044    -1.571066     1.451437     397.94
 H      -4.328651    -1.569996     2.252567      26.12
 C      -5.171641    -3.552086     0.558332      84.63
 O      -4.917016    -4.797694    -0.449155     289.39
 H      -4.326500    -5.307751     0.201630      30.06
 H      -6.087972    -2.924101     0.609586      27.82
 H      -5.449936    -4.049958     1.592395      29.31
55
name = lig-etoh-frame_462
 C       2.285263     1.484007    -2.331369      45.26
 H       1.824128     2.264090    -2.952415      21.57
 C       3.644323     1.251635    -0.231157      91.10
 H       3.770610     1.269276     0.799381      15.97
 C       3.985406    -0.080276    -0.782864      19.53
 O       4.742394    -0.907925    -0.072273     238.10
 C       5.357243    -0.733010     1.269835     117.06
 H       4.647563    -1.036053     2.037352      28.50
 H       5.660749     0.312993     1.342495      28.12
 H       6.130919    -1.401244     1.150789      27.14
 C       3.729357    -0.491305    -2.148256      10.54
 O       4.418234    -1.530154    -2.695115     233.75
 H       4.824551    -1.972682    -2.008369      25.34
 C       2.905823     0.403305    -2.925289      42.23
 H       2.889288     0.136909    -3.955931      22.58
 C       2.594290     1.915200    -0.979047      67.05
 C       1.987550     3.281126    -0.521622      96.13
 H       2.400770     4.007420    -1.435963      19.15
 O       2.545611     3.743649     0.786347     230.09
 H       3.549189     3.980509     0.885232      28.64
 C       0.495260     3.449985    -0.346073      50.20
 H       0.358085     2.712835    -1.219306      17.10
 C       0.126339     5.026173    -0.084884      85.12
 O       0.934177     6.017300    -1.036689     144.15
 H       0.491570     6.029326    -1.913908      28.18
 H       0.533762     5.328530     0.938718      25.71
 H      -0.988997     5.274436    -0.180270      23.97
 C      -1.182078    -0.791405    -0.130193      37.78
 H      -0.574267    -1.804001    -0.071521      16.32
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 C      -3.161302     0.626642    -0.432638      36.61
 H      -4.157672     0.820956    -0.898103      16.93
 C      -2.418934     1.711271     0.021509      -4.18
 O      -2.953726     3.042410     0.193208     211.06
 C      -4.172040     3.348227    -0.600037     110.38
 H      -5.032749     2.875616    -0.069207      25.61
 H      -4.264895     4.385849    -0.735726      26.39
 H      -3.874505     2.982194    -1.621245      25.68
 C      -0.935314     1.631005     0.270450       6.94
 O      -0.077086     2.623625     0.902231     145.56
 C      -0.461788     0.282509     0.399803      26.57
 H       0.729501     0.081660     0.474859      16.18
 C      -2.510962    -0.779353    -0.582096      13.26
 C      -3.481346    -1.985498    -0.653785      83.10
 H      -4.373461    -1.676467    -1.212599      20.05
 O      -2.640059    -3.066233    -1.005335     294.22
 H      -3.181010    -3.824902    -1.111435      17.74
 C      -4.112466    -2.460167     0.720490      79.04
 H      -3.234311    -2.833952     1.386779      17.08
 O      -4.800650    -1.526633     1.474789     350.99
 H      -4.333106    -1.560346     2.461349      21.13
 C      -5.202919    -3.627974     0.545541      78.41
 O      -4.902949    -4.794289    -0.441190     338.60
 H      -4.096012    -5.164471     0.126699      25.53
 H      -6.044950    -2.928041     0.178185      27.43
 H      -5.142319    -4.111541     1.495448      28.75
55
name = lig-etoh-frame_463
 C       2.249929     1.494173    -2.355374      40.35
 H       1.767485     2.188886    -3.029146      20.71
 C       3.653790     1.247166    -0.263139      93.72
 H       3.877341     1.480925     0.865951      11.01
 C       3.974219    -0.040382    -0.888400      25.84
 O       4.719764    -0.892007    -0.007522     261.30
 C       5.394819    -0.731085     1.219916      95.19
 H       4.519200    -1.032002     1.851531      26.00
 H       5.806767     0.282452     1.438144      26.97
 H       6.213686    -1.553183     1.026456      24.19
 C       3.701478    -0.477994    -2.127317      19.99
 O       4.464052    -1.507062    -2.723678     198.48
 H       4.733359    -1.947405    -1.766822      19.21
 C       2.934224     0.404794    -2.888477      32.45
 H       3.030809     0.281028    -4.022654      20.46
 C       2.555125     1.932348    -0.984700      80.68
 C       2.080622     3.238614    -0.526359     102.49
 H       2.349452     3.836374    -1.422896      19.17
 O       2.468838     3.730738     0.741799     226.66
 H       3.540119     3.890444     0.749390      26.95
 C       0.462094     3.431595    -0.402418      37.48
 H      -0.154296     3.038720    -1.265685      18.36
 C       0.131144     4.978272    -0.022303      90.64
 O       0.910029     6.015823    -1.034453     140.38
 H       0.244936     5.839351    -1.746588      27.46
 H       0.491949     5.383772     0.862312      26.61
 H      -0.907616     5.321901    -0.305510      24.00
 C      -1.198512    -0.856529    -0.104779      35.83
 H      -0.780179    -1.774830    -0.146026      17.76
 C      -3.129902     0.640565    -0.473402      65.44
 H      -4.147219     0.368989    -0.843993      17.47
 C      -2.438195     1.756044     0.098962      -3.84
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 O      -2.981323     3.025895     0.267323     222.48
 C      -4.063617     3.366607    -0.665246      89.21
 H      -5.017614     2.914499    -0.339678      24.96
 H      -4.338006     4.640384    -0.915847      22.52
 H      -3.969055     2.949597    -1.692751      25.92
 C      -0.945212     1.647713     0.344918      14.48
 O      -0.070970     2.594851     0.864266     178.19
 C      -0.443085     0.369803     0.357590      34.42
 H       0.548147     0.242076     0.389804      18.09
 C      -2.516128    -0.699004    -0.543446       6.23
 C      -3.475090    -2.085877    -0.643132      62.41
 H      -4.206951    -1.729305    -1.527451      17.91
 O      -2.600526    -3.129440    -1.110243     236.45
 H      -3.064610    -4.099658    -1.153715      15.04
 C      -4.067441    -2.508346     0.691409      92.42
 H      -3.213861    -2.605001     1.318680      18.52
 O      -4.806429    -1.454966     1.523743     341.76
 H      -4.392906    -1.280125     2.539585      23.91
 C      -5.202943    -3.689819     0.489973      92.72
 O      -4.871357    -4.762707    -0.407510     357.34
 H      -4.073378    -5.154537    -0.121334      31.00
 H      -6.078529    -3.396422    -0.089631      26.36
 H      -5.207071    -4.134077     1.541138      25.97
55
name = lig-etoh-frame_464
 C       2.242194     1.529035    -2.339561      65.77
 H       1.607927     2.093956    -3.066980      19.90
 C       3.576297     1.220396    -0.334154      11.34
 H       3.973600     1.645032     0.531398      16.26
 C       4.011591     0.052113    -0.829631      42.74
 O       4.690402    -0.901465    -0.024190     252.64
 C       5.425388    -0.735455     1.166507     127.84
 H       4.785068    -0.901800     2.070701      25.66
 H       5.931427     0.186095     1.509188      26.05
 H       6.183218    -1.495925     1.299360      25.05
 C       3.689973    -0.459889    -2.158922      23.47
 O       4.485940    -1.484339    -2.720611     162.71
 H       4.929286    -2.075105    -1.903175      24.35
 C       2.952847     0.399121    -2.897229      68.81
 H       2.997192     0.419119    -4.027726      20.96
 C       2.572749     1.896440    -0.997896      59.94
 C       2.087376     3.223114    -0.525062      92.55
 H       2.343610     4.066016    -1.411764      17.53
 O       2.404552     3.720756     0.703264     246.42
 H       3.456265     3.701611     0.729081      25.08
 C       0.425210     3.429651    -0.430311      50.27
 H      -0.463358     3.580655    -1.135458      15.23
 C       0.167446     4.950463    -0.035161      85.17
 O       0.855672     5.973808    -1.012401     162.11
 H       0.159902     5.744955    -1.802532      25.62
 H       0.444404     5.252695     1.074084      24.98
 H      -0.891357     5.142618    -0.196759      25.32
 C      -1.205388    -0.847076    -0.066545      37.19
 H      -0.796440    -1.992617    -0.171628      14.72
 C      -3.090507     0.596727    -0.512272      79.15
 H      -4.183447     0.504684    -0.609019      23.80
 C      -2.428285     1.799418     0.148114       2.82
 O      -3.018979     3.026982     0.322968     225.62
 C      -3.991372     3.390311    -0.746762     111.64
 H      -4.999507     3.015760    -0.490308      25.46
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 H      -4.129153     4.445086    -0.686752      26.03
 H      -3.863386     2.900970    -1.712203      27.25
 C      -1.018307     1.632712     0.454871       6.29
 O      -0.066553     2.601254     0.783091     186.57
 C      -0.452324     0.369023     0.260418      18.45
 H       0.737178     0.381209     0.482819      12.38
 C      -2.534475    -0.636038    -0.460953      19.61
 C      -3.445774    -2.097818    -0.681973      75.80
 H      -4.067397    -2.019127    -1.536964      18.09
 O      -2.550323    -3.206759    -1.220308     244.50
 H      -3.055255    -4.032189    -1.177692      17.32
 C      -4.075834    -2.528897     0.696822      78.74
 H      -3.091295    -2.840442     1.288400      15.91
 O      -4.819930    -1.382924     1.543933     348.57
 H      -4.266115    -1.241075     2.322725      26.33
 C      -5.154121    -3.741768     0.460682     106.72
 O      -4.822440    -4.746626    -0.397885     336.52
 H      -3.986776    -5.325371    -0.143903      29.40
 H      -6.220845    -3.568983     0.034816      24.79
 H      -5.633616    -4.008653     1.455541      24.45
55
name = lig-etoh-frame_465
 C       2.262041     1.532743    -2.327002      44.06
 H       1.505234     2.040608    -2.881095      21.26
 C       3.486902     1.219230    -0.373113      71.72
 H       4.081258     1.747151     0.437243      22.09
 C       4.076682     0.058834    -0.756484      53.11
 O       4.674614    -0.923515    -0.072052     249.44
 C       5.453328    -0.728754     1.183793     119.22
 H       4.975899    -0.772489     2.195890      25.83
 H       6.001122     0.252122     1.215424      25.87
 H       6.206538    -1.565131     1.352614      24.14
 C       3.744420    -0.445155    -2.152563      17.60
 O       4.494834    -1.467987    -2.707907     245.32
 H       5.066937    -1.971805    -2.218943      30.35
 C       2.925368     0.441254    -2.954509      57.07
 H       2.868835     0.330645    -4.017919      21.06
 C       2.564779     1.894300    -1.065581      31.37
 C       1.987264     3.250765    -0.598133      98.85
 H       2.330316     4.123187    -1.165485      17.69
 O       2.367447     3.701340     0.703346     281.81
 H       3.363334     3.751526     0.867487      27.72
 C       0.377195     3.470217    -0.422680      73.51
 H      -0.300296     3.441896    -1.272865      20.25
 C       0.222892     4.960564    -0.032179     108.85
 O       0.762092     5.889406    -0.982485     265.49
 H       0.430351     5.850265    -1.848758      31.49
 H       0.451066     5.028958     0.968713      27.43
 H      -0.956786     4.937134     0.065357      24.25
 C      -1.176333    -0.818587    -0.033450      51.40
 H      -0.795857    -1.736819    -0.083195      17.43
 C      -3.088586     0.623017    -0.493333      45.89
 H      -4.158029     0.934209    -0.435563      19.32
 C      -2.409501     1.784982     0.158164       0.73
 O      -3.065098     3.034913     0.352964     212.66
 C      -3.949454     3.363847    -0.783581      84.67
 H      -4.982628     3.070407    -0.511302      24.00
 H      -3.884190     4.675131    -0.585463      21.76
 H      -3.480507     2.959413    -1.767771      23.77
 C      -1.102583     1.605128     0.537334      -5.65
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 O      -0.071118     2.636282     0.688695     191.94
 C      -0.437360     0.298518     0.176810      24.42
 H       0.545803     0.382853     0.494973      14.82
 C      -2.549338    -0.688526    -0.384483      14.96
 C      -3.377855    -2.059620    -0.722927      55.12
 H      -4.286913    -2.118368    -1.533304      16.45
 O      -2.494706    -3.256937    -1.302604     206.60
 H      -3.157100    -3.962158    -1.232213      16.22
 C      -4.112504    -2.539733     0.718475      88.39
 H      -3.370466    -3.099082     1.225400      19.55
 O      -4.824640    -1.350939     1.510299     318.82
 H      -3.890949    -1.262656     2.211855      17.77
 C      -5.162621    -3.733471     0.489030     105.39
 O      -4.737163    -4.783521    -0.428140     354.51
 H      -4.107335    -5.336209     0.140183      30.98
 H      -6.055503    -3.213206     0.115011      28.13
 H      -5.654725    -4.047511     1.431359      27.64
55
name = lig-etoh-frame_466
 C       2.265874     1.499133    -2.382575      52.94
 H       1.410943     2.088725    -2.797470      20.87
 C       3.472272     1.237136    -0.316540      81.44
 H       3.925532     1.747235     0.531181      22.79
 C       4.094354     0.001247    -0.787113      25.99
 O       4.701839    -0.975218    -0.071485     253.37
 C       5.505571    -0.700536     1.216678      99.56
 H       4.824365    -0.592796     2.097927      24.22
 H       6.007558     0.195755     0.814858      24.57
 H       6.157124    -1.604274     1.091999      22.96
 C       3.827994    -0.380203    -2.116293      23.18
 O       4.470118    -1.445331    -2.728509     155.92
 H       5.428407    -1.875597    -2.202363      21.16
 C       2.917185     0.459407    -2.992945      58.43
 H       2.635925     0.061512    -4.083929      18.97
 C       2.508727     1.977189    -1.126117      25.38
 C       1.863314     3.288387    -0.648557     100.67
 H       2.298729     4.160742    -1.384897      17.98
 O       2.335061     3.666304     0.741559     266.24
 H       3.403966     3.907802     0.852142      26.09
 C       0.353187     3.500728    -0.441324      72.89
 H       0.042887     2.999053    -1.479374      18.77
 C       0.190634     4.939177    -0.030858     113.36
 O       0.682020     5.823237    -0.931735     258.31
 H       0.510831     5.732907    -1.926949      28.37
 H       0.813109     5.086452     0.984621      23.69
 H      -0.852124     5.041941     0.186232      25.87
 C      -1.179852    -0.809762    -0.025161      33.11
 H      -0.570980    -1.843293    -0.010802      15.62
 C      -3.110265     0.686093    -0.400623      36.83
 H      -4.146454     1.009261    -0.544734      20.14
 C      -2.419140     1.750031     0.148297       5.55
 O      -3.096928     3.012252     0.367363     236.54
 C      -3.899301     3.387930    -0.772932     121.79
 H      -4.945130     3.082142    -0.693518      26.25
 H      -3.758662     4.439329    -0.783877      26.68
 H      -3.392197     3.101080    -1.613229      28.69
 C      -1.083812     1.565378     0.543548       1.12
 O      -0.103508     2.665709     0.619599     182.77
 C      -0.444719     0.309947     0.169281      27.50
 H       0.676665     0.209012     0.416626      14.58
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 C      -2.590413    -0.771305    -0.352833      11.06
 C      -3.337328    -2.034659    -0.740936      62.12
 H      -4.170461    -1.825931    -1.318603      21.17
 O      -2.459751    -3.263917    -1.338030     156.58
 H      -3.305518    -3.956610    -1.343011      13.01
 C      -4.166308    -2.554301     0.719382      82.55
 H      -3.425159    -3.135156     1.438465      15.65
 O      -4.757436    -1.373846     1.454275     402.73
 H      -4.192619    -1.159821     2.105980      30.78
 C      -5.215310    -3.657586     0.512497      70.98
 O      -4.651399    -4.823104    -0.441926     278.94
 H      -4.197031    -5.262304     0.291274      27.06
 H      -5.873945    -2.935697    -0.076420      25.77
 H      -5.363851    -4.247382     1.492826      27.25
55
name = lig-etoh-frame_467
 C       2.217753     1.494361    -2.472441      52.98
 H       1.442281     2.000793    -3.042565      21.95
 C       3.467390     1.259270    -0.267295      77.94
 H       3.661658     1.640029     0.761146      14.72
 C       4.057523    -0.013419    -0.820540      14.27
 O       4.744290    -1.046309    -0.042787     251.55
 C       5.539366    -0.664424     1.169872      98.87
 H       4.814613    -0.430015     1.940930      25.74
 H       6.152015     0.193594     0.832160      27.89
 H       6.131413    -1.563233     1.166732      24.57
 C       3.894020    -0.286343    -2.149602      23.19
 O       4.467295    -1.439696    -2.748917     240.27
 H       5.214417    -1.566751    -2.243176      24.97
 C       2.942347     0.399134    -3.011643      33.74
 H       2.565033    -0.053075    -3.835386      21.26
 C       2.495638     2.040255    -1.115592      55.99
 C       1.819388     3.351814    -0.642463     112.51
 H       2.064117     3.992037    -1.531070      21.69
 O       2.330457     3.633334     0.772564     281.31
 H       3.210736     3.854505     0.647232      31.88
 C       0.347825     3.456663    -0.517221      80.43
 H       0.086089     3.005983    -1.429243      21.38
 C       0.116991     4.890836     0.014383     106.04
 O       0.635245     5.825637    -0.920787     206.38
 H       0.346119     5.372989    -1.820335      28.20
 H       0.898696     5.069839     0.663177      25.65
 H      -0.940276     5.298435     0.353738      24.12
 C      -1.219768    -0.875282    -0.040841      31.93
 H      -0.602508    -1.736005    -0.010410      17.86
 C      -3.157191     0.658758    -0.292536      44.53
 H      -4.165412     0.736418    -0.757259      19.49
 C      -2.435592     1.740356     0.161065       0.28
 O      -3.103631     2.958297     0.382235     246.87
 C      -3.848439     3.409553    -0.746160      96.33
 H      -4.925531     3.084113    -0.905484      24.70
 H      -3.821267     4.713346    -0.876111      22.92
 H      -3.364182     2.998117    -1.749127      25.06
 C      -0.977457     1.557831     0.465124      21.88
 O      -0.164004     2.672885     0.600652     222.83
 C      -0.427598     0.372642     0.238748      39.07
 H       0.646607     0.090543     0.169258      15.08
 C      -2.595049    -0.785517    -0.342828      10.93
 C      -3.310002    -2.049291    -0.694309      45.11
 H      -4.144478    -1.488218    -1.424138      18.67
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 O      -2.492590    -3.228471    -1.323157     231.91
 H      -3.113803    -3.900262    -1.424956      18.23
 C      -4.146893    -2.570444     0.756971      89.47
 H      -3.395699    -2.813982     1.433433      20.13
 O      -4.703096    -1.431671     1.351533     353.53
 H      -4.252613    -1.080309     2.322698      23.74
 C      -5.243878    -3.574008     0.484502      95.70
 O      -4.594945    -4.820221    -0.434905     267.91
 H      -4.005756    -5.317470     0.320826      23.03
 H      -6.092477    -3.231171    -0.118931      27.56
 H      -5.397593    -4.122260     1.357454      27.51
55
name = lig-etoh-frame_468
 C       2.189429     1.510214    -2.520622      32.99
 H       1.520904     1.870064    -3.329869      19.60
 C       3.436048     1.271564    -0.267243      69.48
 H       3.369605     1.368093     0.856372      13.59
 C       4.017773     0.024313    -0.775693      12.54
 O       4.771629    -1.089357    -0.037085     256.28
 C       5.561264    -0.623331     1.061650     106.59
 H       4.930430    -0.289225     1.957548      27.61
 H       6.306505     0.215726     1.055359      27.75
 H       6.142292    -1.517397     1.612849      25.56
 C       3.932307    -0.229628    -2.253966      13.43
 O       4.449985    -1.412420    -2.769703     141.68
 H       5.271921    -1.613130    -2.120877      21.01
 C       2.957392     0.359492    -2.968321      44.95
 H       2.549911    -0.276194    -3.913265      20.31
 C       2.520070     2.028587    -1.108514      57.03
 C       1.843340     3.360401    -0.592619     103.97
 H       2.022676     4.186030    -1.469613      19.97
 O       2.320783     3.608224     0.762762     225.58
 H       3.395808     3.812975     0.568880      25.89
 C       0.315389     3.395539    -0.554456      74.22
 H      -0.308526     3.228673    -1.554314      18.93
 C       0.024963     4.874514     0.049488      95.41
 O       0.584237     5.844028    -0.968682     242.42
 H       0.178246     5.469626    -1.715856      33.48
 H       0.808586     4.870784     0.920397      24.08
 H      -0.879361     5.170522     0.454025      26.13
 C      -1.242926    -0.870685    -0.043298      45.22
 H      -0.710084    -1.872600    -0.090692      18.45
 C      -3.207947     0.530214    -0.209101      48.20
 H      -4.148584     0.518920    -0.780451      17.13
 C      -2.437152     1.714473     0.194719     -12.77
 O      -3.098679     2.910029     0.394901     251.53
 C      -3.798357     3.455765    -0.783907     117.50
 H      -4.825052     3.102401    -0.804853      26.21
 H      -3.947558     4.524327    -0.720436      26.44
 H      -3.408615     3.062832    -1.640643      29.22
 C      -0.920853     1.615274     0.341461       0.59
 O      -0.223137     2.680841     0.614746     230.19
 C      -0.407942     0.305555     0.292756      41.54
 H       0.651359     0.251950     0.102691      18.59
 C      -2.540821    -0.751215    -0.323663      23.51
 C      -3.348451    -2.065240    -0.643824      76.15
 H      -3.974120    -1.765840    -1.402343      22.04
 O      -2.546272    -3.133562    -1.267128     247.23
 H      -3.151559    -3.980344    -1.407531      15.93
 C      -4.082576    -2.549077     0.751588      72.38
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 H      -3.148003    -2.890773     1.405531      19.08
 O      -4.678306    -1.450110     1.265842     346.27
 H      -4.307280    -1.376231     2.228131      25.17
 C      -5.224607    -3.559563     0.410090      84.56
 O      -4.558520    -4.787456    -0.398362     315.99
 H      -3.857406    -5.194610     0.089841      29.31
 H      -6.258088    -3.540680    -0.051549      25.23
 H      -5.739965    -3.968603     1.432643      24.68
55
name = lig-etoh-frame_469
 C       2.226203     1.509600    -2.512210      30.00
 H       1.568107     1.902769    -3.309381      19.18
 C       3.380707     1.226555    -0.283610      56.48
 H       3.227655     1.264405     0.756314      17.86
 C       4.000938     0.068469    -0.758957       6.05
 O       4.785026    -1.076610    -0.060852     256.34
 C       5.593955    -0.592071     1.042172     121.31
 H       4.967822    -0.162813     1.814952      29.24
 H       6.372597     0.178042     0.892666      28.41
 H       5.973028    -1.338365     1.644287      28.70
 C       3.978945    -0.228679    -2.263742      -0.39
 O       4.459374    -1.374514    -2.780388     167.27
 H       5.138182    -1.966709    -2.126789      19.98
 C       2.892753     0.357959    -2.963200      58.39
 H       2.748150    -0.154355    -3.829447      23.39
 C       2.527365     1.995441    -1.167018      43.74
 C       1.886589     3.315944    -0.580665      99.87
 H       2.155304     4.324338    -1.008314      18.98
 O       2.343411     3.599064     0.724433     298.41
 H       3.298155     3.666017     0.862233      30.71
 C       0.242564     3.396634    -0.542439      91.82
 H      -0.453663     3.450437    -1.352515      19.90
 C       0.014776     4.866332     0.063653      82.61
 O       0.516705     5.860659    -0.996862     186.17
 H      -0.063900     5.765056    -1.912514      25.25
 H       0.419501     4.804466     1.053831      25.54
 H      -1.150744     4.936300     0.412035      22.97
 C      -1.160519    -0.839082    -0.017133      56.54
 H      -0.908018    -1.935674    -0.213586      17.40
 C      -3.214268     0.408381    -0.146480      46.10
 H      -4.237700     0.522499    -0.515061      19.06
 C      -2.435656     1.634080     0.210380      -5.68
 O      -3.085169     2.884055     0.400725     223.94
 C      -3.784545     3.455754    -0.788745      86.06
 H      -4.820902     3.041235    -0.616236      22.96
 H      -3.871678     4.729981    -0.563272      22.62
 H      -3.279044     3.201732    -1.788240      24.67
 C      -0.994878     1.596859     0.221900      -4.02
 O      -0.253518     2.708897     0.632695     219.22
 C      -0.392991     0.206070     0.307544      35.79
 H       0.756519     0.355899     0.246588      16.02
 C      -2.536870    -0.736183    -0.308112      26.39
 C      -3.384101    -2.069469    -0.584238      75.53
 H      -4.255840    -2.020842    -1.463096      16.76
 O      -2.591821    -3.035866    -1.193880     245.99
 H      -3.238500    -3.842589    -1.234470      14.88
 C      -3.995965    -2.545388     0.664081     101.08
 H      -3.312935    -3.142593     1.207285      21.94
 O      -4.679403    -1.432407     1.225807     367.11
 H      -4.354880    -1.444815     2.118114      28.91
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 C      -5.187619    -3.655949     0.373813      85.45
 O      -4.557638    -4.725863    -0.363547     360.73
 H      -3.709982    -5.038804     0.161040      27.30
 H      -6.058673    -3.355202    -0.270559      27.09
 H      -5.648205    -3.800110     1.310664      28.01
55
name = lig-etoh-frame_470
 C       2.285445     1.512093    -2.481150      34.49
 H       1.552836     2.098835    -3.012775      18.48
 C       3.303966     1.150282    -0.317923      51.51
 H       3.207351     1.401068     0.809878      15.38
 C       4.037406     0.054605    -0.813337      23.13
 O       4.782074    -1.010130    -0.100478     250.31
 C       5.606384    -0.533616     1.058992      78.46
 H       4.874292     0.125211     1.646259      26.26
 H       6.383335     0.066642     0.508992      26.08
 H       5.987054    -1.576139     1.551406      24.62
 C       3.973275    -0.233830    -2.167519      11.78
 O       4.496272    -1.373998    -2.796237     246.25
 H       4.878800    -1.935721    -2.235115      25.31
 C       2.865040     0.360151    -2.952515      73.36
 H       2.748856     0.003458    -4.081625      24.47
 C       2.515992     1.978368    -1.238836      34.51
 C       1.919730     3.259878    -0.598528      90.12
 H       2.304105     4.256908    -1.103943      18.88
 O       2.348574     3.575963     0.737455     298.55
 H       3.370456     3.569187     0.892701      28.01
 C       0.211208     3.485013    -0.451533      76.80
 H      -0.421683     3.329822    -1.397528      18.45
 C      -0.042555     4.856533     0.028253     104.64
 O       0.431892     5.876374    -0.995267     229.24
 H      -0.179104     5.939403    -1.756100      29.23
 H       0.391897     5.080224     1.061875      25.34
 H      -1.075487     4.818224    -0.017706      24.47
 C      -1.099807    -0.888547    -0.016737      41.38
 H      -0.745702    -1.858027    -0.184325      19.25
 C      -3.213340     0.395192    -0.093126      42.82
 H      -4.328497     0.541856    -0.038484      17.89
 C      -2.449426     1.546004     0.194131      15.71
 O      -3.055987     2.857458     0.395154     230.07
 C      -3.795530     3.460146    -0.745970     109.59
 H      -4.797204     3.082817    -0.733904      25.40
 H      -3.667852     4.506225    -0.469278      25.37
 H      -3.324686     3.384221    -1.714022      26.84
 C      -1.102851     1.495360     0.167140       6.20
 O      -0.291899     2.701820     0.634239     179.09
 C      -0.340794     0.229356     0.295630      31.69
 H       0.673985     0.141816     0.523100      17.34
 C      -2.559929    -0.791263    -0.300953      26.05
 C      -3.427823    -2.012102    -0.597263     101.72
 H      -4.335443    -1.826922    -1.093297      22.38
 O      -2.603686    -2.980196    -1.129412     291.61
 H      -3.192452    -3.703433    -1.147805      19.41
 C      -4.005101    -2.582223     0.571490      85.61
 H      -3.345819    -3.240576     1.272974      18.30
 O      -4.685750    -1.415754     1.210242     319.79
 H      -4.342793    -1.294624     2.310862      21.39
 C      -5.127281    -3.702811     0.318165      68.37
 O      -4.549448    -4.690530    -0.333965     379.92
 H      -3.843178    -4.982691     0.348234      26.52
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 H      -5.654160    -3.058353    -0.448938      27.45
 H      -5.514373    -3.926734     1.419974      27.55
55
name = lig-etoh-frame_471
 C       2.307514     1.536713    -2.493296      50.55
 H       1.520454     2.231641    -2.908933      16.68
 C       3.220276     1.090768    -0.343045      54.58
 H       3.333116     1.476303     0.618872      21.29
 C       4.098525     0.010225    -0.835277      37.14
 O       4.761012    -0.919758    -0.140794     266.06
 C       5.594812    -0.484308     1.041915     119.84
 H       5.107935     0.271505     1.604546      27.28
 H       6.427552    -0.103650     0.456482      25.69
 H       5.905016    -1.368287     1.395796      27.41
 C       3.885633    -0.270784    -2.144301      24.37
 O       4.530836    -1.357293    -2.828499     174.27
 H       4.880305    -2.061217    -1.983404      20.17
 C       2.907058     0.340478    -2.966500      53.88
 H       2.716486     0.240597    -4.004789      24.46
 C       2.527321     1.959452    -1.185016      28.84
 C       1.925917     3.247281    -0.626303      81.12
 H       2.283912     3.886143    -1.534446      21.60
 O       2.354160     3.535460     0.783587     304.37
 H       3.406554     3.578294     0.630368      26.26
 C       0.247583     3.537759    -0.376089      69.42
 H      -0.057736     3.132214    -1.364680      17.87
 C      -0.110874     4.902559    -0.045243     112.17
 O       0.355012     5.902648    -0.957944     238.93
 H      -0.280593     5.865963    -1.661731      30.35
 H       0.334495     5.382343     0.826595      24.52
 H      -1.277364     4.959635    -0.221607      21.56
 C      -1.110442    -0.958426    -0.047221      18.79
 H      -0.355574    -1.906029    -0.059340      16.56
 C      -3.238452     0.427053    -0.033719      53.71
 H      -4.248344     0.430397     0.303944      17.83
 C      -2.509997     1.516746     0.153926      15.33
 O      -3.018141     2.807397     0.379644     237.82
 C      -3.792501     3.441092    -0.669527      94.04
 H      -4.898503     3.171595    -0.907773      24.48
 H      -3.688485     4.668285    -0.341602      22.66
 H      -3.318126     3.331069    -1.654006      25.59
 C      -1.080108     1.406951     0.195264      17.15
 O      -0.359636     2.643900     0.622885     170.71
 C      -0.334839     0.285677     0.258703      35.75
 H       0.675274     0.036239     0.782547      16.51
 C      -2.547644    -0.856739    -0.282228      31.30
 C      -3.439729    -1.918038    -0.620382      65.25
 H      -4.395717    -1.353889    -1.151612      20.70
 O      -2.582667    -2.958071    -1.113702     196.96
 H      -3.132242    -3.907914    -1.194909      14.05
 C      -4.073768    -2.636728     0.628148     102.30
 H      -3.253790    -2.890858     1.284876      22.55
 O      -4.694413    -1.417797     1.239010     405.13
 H      -4.321401    -1.260307     2.036552      32.24
 C      -5.084558    -3.608158     0.300059     100.45
 O      -4.504682    -4.738973    -0.331357     361.31
 H      -3.981275    -5.216236     0.350176      29.39
 H      -5.712889    -3.019005    -0.423483      27.56
 H      -5.563872    -4.004813     1.131501      27.12
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name = lig-etoh-frame_472
 C       2.306115     1.574899    -2.506662      44.55
 H       1.644482     2.093354    -3.165822      21.16
 C       3.203592     1.021416    -0.345550      75.58
 H       3.496416     1.439947     0.683146      21.85
 C       4.079813     0.029053    -0.835825      41.92
 O       4.754345    -0.852579    -0.141867     259.29
 C       5.583345    -0.423591     0.950755     118.68
 H       5.317588     0.385264     1.743814      23.57
 H       6.597113    -0.094599     0.626924      24.44
 H       5.831644    -1.425198     1.618248      23.75
 C       3.790516    -0.370256    -2.230305      21.95
 O       4.566530    -1.352750    -2.824359     236.87
 H       4.944156    -1.890428    -2.100588      26.23
 C       2.937034     0.393306    -2.980402      47.44
 H       2.775384     0.129690    -4.063016      21.09
 C       2.516241     1.916389    -1.089583      47.16
 C       1.888166     3.244628    -0.615895      80.90
 H       2.155045     3.897544    -1.561830      20.51
 O       2.394470     3.500481     0.780553     309.14
 H       3.307483     3.688452     0.725582      30.07
 C       0.345079     3.469623    -0.357472      66.38
 H       0.034852     3.188423    -1.374769      20.38
 C      -0.223366     5.009105    -0.121063     108.75
 O       0.291157     5.953968    -0.942733     263.76
 H      -0.238427     5.753375    -1.891849      24.40
 H       0.100493     5.325678     0.905972      24.88
 H      -1.274325     5.064219     0.018494      25.05
 C      -1.112474    -0.994686    -0.078388      58.85
 H      -0.511221    -1.774544    -0.023734      20.41
 C      -3.259579     0.393183     0.021954      45.99
 H      -4.318309     0.282206     0.384675      15.54
 C      -2.522940     1.551121     0.104516       9.02
 O      -2.996658     2.756173     0.369069     256.33
 C      -3.786352     3.451742    -0.599149     114.16
 H      -4.815849     3.198609    -0.760165      26.71
 H      -3.888776     4.534739    -0.347647      25.80
 H      -3.227606     3.234437    -1.539066      25.55
 C      -1.003793     1.427183     0.259743       3.85
 O      -0.429434     2.577203     0.614152     206.41
 C      -0.364326     0.227680     0.224722      48.05
 H       0.558180     0.273841     0.749762      17.84
 C      -2.481140    -0.851257    -0.228325      26.14
 C      -3.476231    -1.882450    -0.630478      78.40
 H      -4.061898    -1.399531    -1.356248      22.63
 O      -2.562337    -2.970849    -1.152599     253.88
 H      -3.017507    -3.788847    -1.169579      19.32
 C      -4.097118    -2.561870     0.735228      95.23
 H      -3.159340    -2.745994     1.297517      23.20
 O      -4.739155    -1.440851     1.268897     362.00
 H      -4.121880    -1.252085     2.161255      22.22
 C      -5.086911    -3.525245     0.278843      94.25
 O      -4.451365    -4.816437    -0.365020     279.05
 H      -4.077604    -5.488111     0.363598      26.46
 H      -5.947833    -3.209474    -0.374443      26.01
 H      -5.891130    -3.944406     1.052721      24.77
55
name = lig-etoh-frame_473
 C       2.318042     1.593328    -2.480082      50.51
 H       1.793369     2.025019    -3.371457      21.91
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 C       3.257691     0.980414    -0.268926      50.33
 H       3.507006     1.210039     0.740984      19.83
 C       3.967051     0.057089    -0.927289      12.68
 O       4.782132    -0.816509    -0.103522     275.35
 C       5.619423    -0.392039     0.918936     133.83
 H       5.252913     0.375423     1.567601      27.73
 H       6.655463    -0.136548     0.698441      26.12
 H       5.583668    -1.159198     1.597487      28.42
 C       3.743016    -0.460897    -2.272006      13.95
 O       4.592522    -1.351981    -2.829560     215.77
 H       5.157839    -1.848763    -2.132941      23.75
 C       2.937266     0.474237    -3.038245      59.46
 H       2.854201    -0.034399    -4.043712      21.11
 C       2.432493     1.886782    -1.089520      33.29
 C       1.853521     3.230026    -0.537695      94.37
 H       2.015515     4.194937    -1.177583      19.22
 O       2.437701     3.482081     0.750027     266.58
 H       3.454085     3.839286     0.898308      24.75
 C       0.395643     3.376778    -0.395534      60.77
 H      -0.165778     3.279093    -1.383938      20.19
 C      -0.310731     5.061641    -0.101956      88.29
 O       0.223758     6.031112    -0.997561     281.98
 H       0.146306     5.799388    -1.903194      29.88
 H      -0.054099     5.112400     0.979598      23.52
 H      -1.464500     4.967162     0.067270      22.98
 C      -1.100833    -0.962466    -0.094182      60.71
 H      -0.682594    -2.117750    -0.121956      16.89
 C      -3.236559     0.339058     0.073045      45.46
 H      -4.304161     0.252170     0.145157      16.50
 C      -2.460252     1.542329     0.063035       7.54
 O      -3.004268     2.754288     0.391968     245.99
 C      -3.779021     3.440258    -0.556479     101.26
 H      -4.840462     2.969683    -0.503666      23.81
 H      -3.877516     4.668511    -0.249874      23.41
 H      -3.297996     3.407371    -1.530194      25.93
 C      -1.016092     1.459415     0.288902       5.29
 O      -0.443314     2.570509     0.620615     201.37
 C      -0.403887     0.144963     0.208764      39.23
 H       0.670890     0.316755     0.549614      16.65
 C      -2.467865    -0.805454    -0.167752      28.11
 C      -3.428046    -1.933668    -0.613491      72.53
 H      -4.012676    -1.684311    -1.637387      18.72
 O      -2.545261    -2.973412    -1.208828     236.39
 H      -3.116053    -3.834484    -1.115492      15.65
 C      -4.080145    -2.411458     0.756938      91.16
 H      -3.250761    -2.967547     1.310372      22.17
 O      -4.804478    -1.451172     1.369739     358.05
 H      -4.157995    -1.155742     2.186949      24.21
 C      -5.158492    -3.573840     0.280022      74.61
 O      -4.424986    -4.870433    -0.404159     273.95
 H      -4.139638    -5.358208     0.361747      28.36
 H      -5.849020    -3.265675    -0.595919      26.54
 H      -5.793634    -3.774951     1.099094      26.73
55
name = lig-etoh-frame_474
 C       2.329815     1.586294    -2.471482      35.72
 H       1.812017     2.255438    -3.153204      22.44
 C       3.263972     1.028488    -0.224148      47.88
 H       3.435579     1.063300     0.878506      16.67
 C       3.885929    -0.008315    -1.002017       4.74
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 O       4.802106    -0.798593    -0.107975     253.82
 C       5.654196    -0.344354     0.935538      87.95
 H       5.105408     0.609763     1.326065      25.39
 H       6.710929    -0.228073     0.603111      24.20
 H       5.515613    -1.236440     1.735764      23.67
 C       3.711464    -0.459497    -2.273360      23.53
 O       4.606532    -1.373192    -2.848461     196.24
 H       5.434418    -1.729689    -2.148350      20.53
 C       2.971017     0.460618    -3.093824      71.64
 H       2.772900     0.202183    -4.118244      21.71
 C       2.351437     1.871689    -1.105350      26.86
 C       1.857477     3.222828    -0.434749     110.23
 H       2.054149     4.248165    -0.993001      18.80
 O       2.486080     3.478203     0.763130     277.52
 H       3.417484     3.776819     0.656448      27.30
 C       0.311149     3.335422    -0.442381      65.03
 H      -0.165891     3.160209    -1.357873      19.94
 C      -0.374874     5.030042    -0.054349      74.93
 O       0.166556     6.120839    -1.023182     231.89
 H       0.268960     5.715445    -1.983005      27.06
 H       0.040686     5.236051     0.929291      22.72
 H      -1.409875     4.826684    -0.304490      22.17
 C      -1.088140    -0.993017    -0.102600      43.37
 H      -0.932548    -1.983324    -0.302579      19.96
 C      -3.170917     0.338651     0.096488      55.83
 H      -4.257530     0.377246    -0.168697      17.06
 C      -2.395799     1.501739     0.067501      19.35
 O      -3.005916     2.779096     0.438641     231.28
 C      -3.812763     3.441669    -0.521713     117.93
 H      -4.736646     2.917431    -0.445330      25.44
 H      -3.817499     4.488893    -0.113439      24.96
 H      -3.495559     3.561706    -1.594935      25.88
 C      -1.093769     1.405031     0.269698      14.89
 O      -0.386357     2.627263     0.640783     189.12
 C      -0.381433     0.160904     0.229503      42.01
 H       0.738339     0.030744     0.158540      17.40
 C      -2.530991    -0.800871    -0.149943      26.24
 C      -3.316342    -1.994204    -0.614374      96.15
 H      -4.094564    -1.843153    -1.303639      21.99
 O      -2.540592    -2.998824    -1.248345     252.44
 H      -3.126184    -3.872730    -1.075551      13.11
 C      -4.085413    -2.368947     0.672421      90.58
 H      -3.489429    -2.994091     1.322894      20.04
 O      -4.874703    -1.433799     1.516480     368.48
 H      -4.372718    -1.092413     2.221291      31.02
 C      -5.196891    -3.642663     0.248543      59.16
 O      -4.440609    -4.873589    -0.425464     260.78
 H      -3.989691    -5.262107     0.412122      24.50
 H      -5.616089    -3.246969    -0.660111      26.63
 H      -5.700567    -3.854644     1.284092      26.27
55
name = lig-etoh-frame_475
 C       2.336264     1.566170    -2.480944      61.92
 H       1.777429     2.435490    -2.857875      15.54
 C       3.216739     1.086061    -0.281840      81.45
 H       3.268153     1.068702     0.826369      15.88
 C       3.853362    -0.074686    -0.909577      -2.50
 O       4.806396    -0.813917    -0.172694     229.85
 C       5.642194    -0.290420     0.978853     114.50
 H       5.399111     0.738640     1.168281      28.96
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 H       6.662240    -0.304480     0.570943      26.06
 H       5.632559    -0.997624     1.756751      28.26
 C       3.721338    -0.428485    -2.319547      24.45
 O       4.621162    -1.400858    -2.862984     226.07
 H       5.238443    -1.578442    -2.272674      25.32
 C       2.986310     0.427556    -3.127652      56.15
 H       2.745720     0.555763    -4.255170      22.92
 C       2.338024     1.865565    -1.052995      45.01
 C       1.841213     3.228675    -0.396826     101.75
 H       2.208849     3.994719    -1.185903      22.19
 O       2.520251     3.471231     0.825813     274.93
 H       3.473489     3.654819     0.496004      27.02
 C       0.186802     3.370036    -0.427037      60.52
 H      -0.061044     2.951198    -1.501780      16.95
 C      -0.365408     4.956445    -0.090664      78.97
 O       0.116777     6.188859    -1.010725     219.15
 H       0.048388     5.660766    -1.893300      26.41
 H      -0.041360     5.444490     0.876325      21.74
 H      -1.389366     4.814959    -0.447772      20.79
 C      -1.148312    -0.987284    -0.097520      23.30
 H      -0.713059    -2.042106    -0.466789      17.27
 C      -3.158844     0.389060     0.067806      54.15
 H      -4.158634     0.571597    -0.312588      15.26
 C      -2.424334     1.516273     0.134057      18.75
 O      -2.972395     2.782866     0.476632     228.37
 C      -3.862187     3.434811    -0.487567     103.62
 H      -4.938652     2.993812    -0.544927      24.66
 H      -3.953661     4.561011     0.034834      23.26
 H      -3.582100     3.495809    -1.542669      26.04
 C      -1.041551     1.372617     0.267551       1.39
 O      -0.321781     2.659550     0.654493     191.36
 C      -0.326109     0.164630     0.221486      44.97
 H       0.690148    -0.001588    -0.013462      18.60
 C      -2.537644    -0.870224    -0.180150      24.67
 C      -3.248816    -2.023428    -0.593906      86.77
 H      -4.265469    -1.629187    -1.130266      19.62
 O      -2.536716    -3.057176    -1.264954     261.49
 H      -3.017044    -3.856141    -1.157182      18.11
 C      -4.143602    -2.447806     0.623678      69.50
 H      -3.479746    -2.898330     1.449302      19.10
 O      -4.955057    -1.431456     1.610211     198.97
 H      -4.230850    -1.075645     2.486623      18.23
 C      -5.164072    -3.685154     0.215039      77.08
 O      -4.474366    -4.843447    -0.404694     315.80
 H      -3.753734    -5.207181     0.248208      25.79
 H      -5.834267    -3.215378    -0.653635      25.01
 H      -5.702697    -4.030141     1.068319      27.19
55
name = lig-etoh-frame_476
 C       2.328402     1.560337    -2.441591      49.22
 H       1.773712     2.368600    -2.992124      18.43
 C       3.173775     1.061561    -0.351421      71.53
 H       3.164528     1.259206     0.704742      13.98
 C       3.830429    -0.103751    -0.785204       8.62
 O       4.812855    -0.847207    -0.237912     238.12
 C       5.630732    -0.226266     0.962443     102.77
 H       5.606782     0.887533     1.208811      27.15
 H       6.649563    -0.373105     0.561249      26.03
 H       5.576093    -0.846600     1.966008      26.21
 C       3.786097    -0.405161    -2.351074     -14.56
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 O       4.587732    -1.407243    -2.895536     112.00
 H       5.318401    -1.643644    -2.019961      16.98
 C       2.941962     0.474284    -3.159258      48.45
 H       2.982618     0.527110    -4.206850      25.59
 C       2.355993     1.864241    -1.013622      37.62
 C       1.805467     3.221030    -0.431313      84.66
 H       2.249714     3.857819    -1.328024      21.19
 O       2.524556     3.468480     0.887277     251.31
 H       3.610057     3.518457     0.716763      25.97
 C       0.145769     3.464649    -0.399733      80.15
 H      -0.030077     3.012410    -1.315952      21.20
 C      -0.323575     4.900753    -0.194068     101.27
 O       0.065564     6.200318    -0.980531     261.77
 H      -0.194340     5.947971    -1.892898      28.98
 H      -0.322981     5.268947     0.823133      25.17
 H      -1.473801     4.940531    -0.243858      21.85
 C      -1.175286    -0.981960    -0.091155      70.98
 H      -0.458355    -1.714155    -0.415585      21.19
 C      -3.191413     0.408594    -0.022471      50.85
 H      -4.251672     0.598782    -0.245665      19.42
 C      -2.442805     1.571547     0.250739      -5.56
 O      -2.940872     2.784274     0.489993     217.15
 C      -3.941191     3.433868    -0.430011     106.81
 H      -4.956494     3.075536    -0.523636      25.70
 H      -4.139822     4.501844    -0.025402      24.71
 H      -3.446313     3.425843    -1.417447      25.68
 C      -0.907572     1.406362     0.304312     -11.35
 O      -0.286124     2.634194     0.668790     216.02
 C      -0.316112     0.136843     0.175683      36.92
 H       0.860070     0.178078     0.006747      15.49
 C      -2.490853    -0.900690    -0.211672      33.39
 C      -3.334760    -2.042245    -0.577374      87.07
 H      -3.954129    -1.529471    -1.262046      21.87
 O      -2.525315    -3.103023    -1.270875     198.60
 H      -3.134482    -4.020984    -1.274970      13.60
 C      -4.211094    -2.601119     0.683750      74.08
 H      -3.452245    -2.853269     1.377314      22.26
 O      -5.000003    -1.440878     1.670426     262.23
 H      -4.302456    -1.429115     2.224935      26.07
 C      -5.118963    -3.682112     0.164779     105.20
 O      -4.492997    -4.802721    -0.385523     338.78
 H      -3.794132    -5.112990     0.160921      31.56
 H      -5.966054    -3.397127    -0.432565      25.78
 H      -5.827824    -4.132008     0.971474      24.39
55
name = lig-etoh-frame_477
 C       2.290389     1.586506    -2.406045      60.91
 H       1.818989     2.106462    -3.181758      22.07
 C       3.169438     0.968862    -0.313916      49.52
 H       3.265435     1.436894     0.724846      13.88
 C       3.802460    -0.125767    -0.804956       6.61
 O       4.843623    -0.872902    -0.240077     242.11
 C       5.644503    -0.185924     0.927604      98.50
 H       5.532002     0.911703     1.067953      27.29
 H       6.654006    -0.500341     0.628748      25.60
 H       5.297162    -0.605339     1.887966      27.43
 C       3.829907    -0.348983    -2.330886     -14.11
 O       4.557601    -1.398634    -2.891268     184.07
 H       5.124999    -1.811344    -2.228664      21.89
 C       2.924137     0.526971    -3.121373      53.32
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 H       3.169822     0.371097    -4.244845      23.91
 C       2.335457     1.879228    -1.073682      51.30
 C       1.804119     3.216102    -0.476194      89.42
 H       2.191511     4.011104    -1.231108      22.62
 O       2.499795     3.465871     0.915382     298.31
 H       3.450306     3.561728     0.965070      29.94
 C       0.226756     3.541810    -0.374872      64.10
 H      -0.246658     3.130890    -1.368603      20.70
 C      -0.348225     4.920743    -0.283363     112.00
 O       0.021023     6.159301    -0.940920     262.50
 H      -0.378480     6.329519    -1.905364      25.91
 H      -0.265158     4.981773     0.869515      24.43
 H      -1.411573     4.875186    -0.242337      24.19
 C      -1.081298    -0.954294    -0.083478      69.06
 H      -0.464768    -1.839460    -0.360716      20.82
 C      -3.199521     0.418960    -0.128341      47.42
 H      -4.325880     0.400763    -0.060450      23.02
 C      -2.394938     1.557041     0.354968     -20.73
 O      -2.939687     2.824954     0.506658     190.53
 C      -3.996017     3.418762    -0.376758      91.44
 H      -4.979085     2.848408    -0.399283      24.26
 H      -4.149180     4.568727    -0.017439      23.36
 H      -3.397291     3.474578    -1.320063      24.09
 C      -0.848729     1.465141     0.362980      -2.14
 O      -0.258620     2.592306     0.696989     190.35
 C      -0.303822     0.172159     0.122223      48.18
 H       0.702273     0.157710     0.164948      19.02
 C      -2.506513    -0.869984    -0.227861      16.90
 C      -3.454792    -2.065776    -0.567889      59.88
 H      -3.930727    -1.672924    -1.586743      18.20
 O      -2.536846    -3.154054    -1.257264     218.02
 H      -3.169072    -3.825389    -1.409787      19.70
 C      -4.270867    -2.693471     0.752175      67.40
 H      -3.384329    -3.116640     1.388448      19.21
 O      -5.032401    -1.502343     1.654139     267.04
 H      -4.164088    -1.570531     2.367510      19.43
 C      -5.152602    -3.695506     0.192410      98.78
 O      -4.491101    -4.777718    -0.411568     317.56
 H      -3.845006    -5.131299     0.363578      25.65
 H      -6.012172    -3.352933    -0.570125      24.90
 H      -5.737590    -4.061774     1.057447      25.83
55
name = lig-etoh-frame_478
 C       2.243142     1.601613    -2.459597      29.78
 H       1.624909     2.155836    -3.240454      19.81
 C       3.137040     0.934588    -0.226836      50.73
 H       3.475962     1.269593     0.713141      16.50
 C       3.824429    -0.165094    -0.916917       3.59
 O       4.881171    -0.877456    -0.199858     240.56
 C       5.634701    -0.170440     0.863549      86.76
 H       5.450744     0.916788     0.714527      27.91
 H       6.678573    -0.557881     0.828136      25.35
 H       5.096758    -0.527453     1.806368      26.72
 C       3.816336    -0.275565    -2.276489      19.02
 O       4.506517    -1.371351    -2.894673     186.03
 H       5.112255    -1.950806    -2.267942      19.84
 C       2.995796     0.516219    -3.032403      53.02
 H       3.006465     0.400228    -4.099176      25.41
 C       2.323034     1.877006    -1.113435      56.80
 C       1.841971     3.246488    -0.493113     101.48
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 H       2.185381     4.207652    -1.105491      22.62
 O       2.414310     3.457447     0.914638     236.35
 H       3.500438     3.760506     0.901547      24.33
 C       0.350845     3.519215    -0.428172      62.19
 H      -0.215678     3.220618    -1.264418      21.09
 C      -0.408643     4.978455    -0.271402      96.53
 O      -0.003119     6.122634    -0.897861     266.79
 H      -0.461125     6.261700    -1.731293      29.30
 H      -0.051227     5.108659     0.735592      24.32
 H      -1.512847     4.626829    -0.499672      21.63
 C      -0.999497    -0.942602    -0.102245      28.84
 H      -0.748016    -2.063829    -0.195064      19.47
 C      -3.155463     0.428019    -0.183827      58.49
 H      -4.196691     0.295618     0.032557      22.86
 C      -2.340389     1.504765     0.393400      -7.96
 O      -2.945483     2.881020     0.546235     186.98
 C      -4.012668     3.384387    -0.325639     103.40
 H      -4.830118     2.661583    -0.283512      25.35
 H      -4.173798     4.499346     0.067214      23.88
 H      -3.667226     3.517560    -1.359278      25.85
 C      -0.926982     1.483112     0.410584      16.93
 O      -0.198900     2.603827     0.742644     171.80
 C      -0.294875     0.263592     0.094089      35.85
 H       0.866035     0.011779     0.301682      17.14
 C      -2.547251    -0.826882    -0.246493      -8.97
 C      -3.513413    -2.073045    -0.585772      63.35
 H      -4.217680    -1.991814    -1.391254      21.41
 O      -2.562787    -3.178480    -1.216385     204.81
 H      -3.257682    -3.843354    -1.526471      18.57
 C      -4.282219    -2.678234     0.793885      77.44
 H      -3.613668    -3.316884     1.315764      20.80
 O      -4.998532    -1.634196     1.607646     361.64
 H      -4.541968    -1.271742     2.438734      26.60
 C      -5.287371    -3.728603     0.247007      87.90
 O      -4.465034    -4.778024    -0.437687     318.21
 H      -4.037922    -5.236871     0.305869      27.47
 H      -5.767262    -3.244519    -0.558537      28.28
 H      -5.786192    -4.081225     1.205555      27.32
55
name = lig-etoh-frame_479
 C       2.207222     1.588948    -2.550974      26.10
 H       1.514772     2.236558    -3.005968      21.73
 C       3.096481     0.922759    -0.228840      50.81
 H       3.545399     1.065707     0.810556      17.73
 C       3.885256    -0.145776    -0.902912      16.66
 O       4.902011    -0.885532    -0.184013     274.49
 C       5.585293    -0.170863     0.796896     106.52
 H       5.627704     0.897657     0.401054      27.67
 H       6.615289    -0.500127     1.013996      25.93
 H       5.039088    -0.287841     1.803283      26.69
 C       3.824255    -0.293451    -2.250303      26.18
 O       4.443060    -1.327021    -2.907585     191.55
 H       5.137688    -1.880955    -2.207805      19.29
 C       3.038239     0.538989    -2.967645      52.86
 H       2.818728     0.380323    -4.042890      21.91
 C       2.349600     1.868943    -1.075739      34.36
 C       1.908064     3.299067    -0.484375     102.16
 H       2.328567     4.229822    -1.045689      22.48
 O       2.338849     3.458712     0.891066     310.89
 H       3.157591     3.774959     0.690993      29.74
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 C       0.426706     3.460562    -0.483242      44.27
 H      -0.002843     2.998185    -1.439561      20.32
 C      -0.457447     4.967068    -0.193353      87.02
 O      -0.010023     6.120208    -0.874536     258.22
 H      -0.445385     6.033654    -1.763385      27.61
 H      -0.227577     5.372336     0.854920      21.86
 H      -1.369672     4.629969    -0.514683      23.03
 C      -1.042766    -0.936296    -0.139271      22.62
 H      -0.754072    -1.934029    -0.040256      22.49
 C      -3.081654     0.437910    -0.168861      65.29
 H      -4.210203     0.479943    -0.021488      24.74
 C      -2.352776     1.510953     0.365750      12.95
 O      -2.929441     2.912318     0.596102     195.39
 C      -4.000770     3.322436    -0.272559     110.17
 H      -4.880481     2.631146    -0.184404      25.76
 H      -4.343228     4.371594     0.208182      24.40
 H      -3.943614     3.474258    -1.411221      25.31
 C      -1.009957     1.497708     0.444129       2.81
 O      -0.127498     2.646283     0.783531     119.93
 C      -0.254291     0.282975     0.101501      22.12
 H       0.744062     0.196064     0.306246      18.93
 C      -2.540865    -0.821127    -0.295772       0.01
 C      -3.499815    -2.103016    -0.566771      58.38
 H      -4.554686    -1.994444    -1.138164      20.48
 O      -2.609656    -3.171677    -1.158574     207.75
 H      -3.247343    -3.950076    -1.537045      15.18
 C      -4.279813    -2.630704     0.808043      86.85
 H      -3.617499    -3.346144     1.431960      19.22
 O      -4.967382    -1.777427     1.540881     394.17
 H      -4.641362    -1.257683     2.260562      31.24
 C      -5.387425    -3.758984     0.311512      65.22
 O      -4.474737    -4.780488    -0.452227     271.52
 H      -4.044601    -5.394814     0.203158      26.49
 H      -5.905585    -3.162958    -0.571057      26.01
 H      -6.082047    -4.194699     1.109530      26.50
55
name = lig-etoh-frame_480
 C       2.208957     1.580581    -2.500862      57.32
 H       1.505441     2.265242    -3.017639      22.21
 C       3.101424     0.914377    -0.286389      55.83
 H       3.217350     1.059305     0.779291      18.50
 C       3.945975    -0.080635    -0.789741      23.24
 O       4.892719    -0.916372    -0.206838     295.16
 C       5.547256    -0.127304     0.762455     124.31
 H       5.848368     0.855270     0.392211      27.00
 H       6.522335    -0.575354     1.010823      25.87
 H       5.017993     0.044364     1.759764      26.50
 C       3.846670    -0.355788    -2.230426      21.74
 O       4.405859    -1.305022    -2.920397     238.80
 H       5.017778    -1.618369    -2.351537      28.02
 C       2.998163     0.603256    -3.006233      52.10
 H       2.837056     0.153822    -4.042778      22.06
 C       2.401795     1.862746    -1.037060      33.05
 C       1.966168     3.319696    -0.462298      91.38
 H       2.509494     4.145010    -1.167839      21.08
 O       2.268538     3.466856     0.860837     265.94
 H       3.275978     3.835885     0.782772      23.15
 C       0.411374     3.413626    -0.504450      42.95
 H       0.232175     2.870998    -1.440850      20.86
 C      -0.424001     4.920874    -0.088231      78.23
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 O      -0.023287     6.131697    -0.884510     250.61
 H      -0.165635     5.861982    -1.911452      26.04
 H      -0.664594     5.179940     0.951687      23.32
 H      -1.557843     4.680838    -0.388665      20.22
 C      -1.141323    -0.886357    -0.173538      46.93
 H      -0.481901    -1.852097    -0.003182      19.91
 C      -3.069531     0.454891    -0.109764      58.34
 H      -4.097470     0.710770    -0.275914      20.79
 C      -2.413878     1.609704     0.313430       5.51
 O      -2.900135     2.903245     0.629579     224.57
 C      -4.025012     3.258343    -0.212846     121.63
 H      -4.934501     2.616332    -0.037385      25.75
 H      -4.573946     4.196751     0.303906      24.99
 H      -3.871041     3.382742    -1.258969      27.47
 C      -0.955261     1.512382     0.460828     -19.65
 O      -0.079085     2.674261     0.791722     135.90
 C      -0.306642     0.258960     0.136752      11.48
 H       0.859561     0.395853     0.287391      14.69
 C      -2.499161    -0.862665    -0.362282      29.07
 C      -3.476017    -2.142725    -0.518252      85.28
 H      -4.331311    -1.706761    -1.009838      23.24
 O      -2.671227    -3.142536    -1.109287     293.45
 H      -3.194355    -3.872128    -1.246686      20.51
 C      -4.235392    -2.704271     0.803977      88.73
 H      -3.491434    -3.120937     1.459819      22.29
 O      -5.000798    -1.864590     1.487921     347.26
 H      -4.279486    -1.274289     2.161971      22.74
 C      -5.413883    -3.768473     0.319343      87.58
 O      -4.540918    -4.781360    -0.458426     288.65
 H      -3.993919    -5.404111     0.183002      26.47
 H      -6.142505    -3.392335    -0.358214      28.01
 H      -6.192048    -4.241908     0.957046      26.08
55
name = lig-etoh-frame_481
 C       2.224300     1.613900    -2.356202      76.54
 H       1.663987     2.180695    -3.116201      23.90
 C       3.134205     0.931300    -0.301267      53.00
 H       2.882376     1.183359     0.762225      18.58
 C       3.984325    -0.055716    -0.790777      18.73
 O       4.865251    -0.938401    -0.213982     289.88
 C       5.568947    -0.074387     0.774769      99.05
 H       6.020694     0.885412     0.305834      24.97
 H       6.369614    -0.790018     1.042087      24.37
 H       4.898631     0.352482     1.624680      24.34
 C       3.783281    -0.292711    -2.183348       6.96
 O       4.388933    -1.316360    -2.953527     152.48
 H       5.332836    -1.714779    -2.364954      20.67
 C       2.968285     0.573103    -3.071176      48.92
 H       2.889027     0.164812    -4.039215      22.73
 C       2.438859     1.875648    -1.049782      47.40
 C       1.983691     3.299116    -0.472497      89.43
 H       2.533991     3.916424    -1.260467      20.90
 O       2.266993     3.509735     0.857322     299.32
 H       3.214836     3.667727     1.220005      26.10
 C       0.372689     3.412522    -0.458051      59.45
 H       0.020822     2.916485    -1.381481      22.53
 C      -0.414400     4.849961    -0.063803      88.29
 O      -0.033653     6.117508    -0.895894     280.47
 H       0.090622     5.834970    -1.772959      31.70
 H      -0.629326     4.904312     1.045244      24.30
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 H      -1.408297     4.715017    -0.320962      24.66
 C      -1.144272    -0.857768    -0.180082      83.49
 H      -0.530145    -1.678512    -0.241847      22.39
 C      -3.103869     0.480477    -0.062155      57.17
 H      -4.104521     0.676265    -0.561081      16.32
 C      -2.385124     1.713320     0.275564      -6.60
 O      -2.888611     2.876804     0.642208     203.97
 C      -4.105933     3.200777    -0.111884     112.96
 H      -4.845983     2.414629     0.006044      26.18
 H      -4.522254     4.208734     0.299174      25.52
 H      -3.651035     3.325605    -1.176850      26.04
 C      -0.867483     1.530223     0.457933      -3.56
 O      -0.059375     2.664745     0.760130     187.70
 C      -0.398794     0.279083     0.200592      53.86
 H       0.697906     0.245288     0.129193      19.05
 C      -2.505290    -0.885718    -0.387499      17.86
 C      -3.433848    -2.127278    -0.443760      83.75
 H      -4.166649    -1.544020    -1.240661      20.03
 O      -2.713225    -3.103319    -1.081899     229.80
 H      -3.371220    -4.008339    -0.911857      13.61
 C      -4.200951    -2.849834     0.763885      92.15
 H      -3.312181    -3.167559     1.435006      21.35
 O      -5.036896    -1.856624     1.495689     407.17
 H      -4.357879    -1.480058     1.915137      29.87
 C      -5.354921    -3.801098     0.293976      81.07
 O      -4.642554    -4.798574    -0.465887     306.34
 H      -4.092281    -5.166043     0.219050      29.57
 H      -6.223455    -3.411051    -0.402512      24.78
 H      -5.932398    -4.340865     1.191785      25.24
55
name = lig-etoh-frame_482
 C       2.265595     1.613877    -2.341412      84.49
 H       1.734192     2.269089    -2.976376      25.67
 C       3.172478     0.979243    -0.244061     110.52
 H       2.890347     1.151656     0.815079      20.58
 C       3.974696    -0.056944    -0.873697      18.79
 O       4.834981    -0.924166    -0.187268     278.36
 C       5.622992    -0.033372     0.789570      95.25
 H       6.106407     0.711578     0.204908      26.94
 H       6.217081    -0.804517     1.308475      24.49
 H       4.899737     0.375580     1.475812      27.00
 C       3.710149    -0.208088    -2.215875      27.90
 O       4.412236    -1.341012    -2.949474     191.96
 H       5.173715    -1.717500    -2.618854      29.17
 C       2.940616     0.512338    -3.031611      56.89
 H       2.834647     0.366441    -4.200540      19.61
 C       2.456838     1.913142    -1.038942      42.48
 C       1.964022     3.235200    -0.501937      83.64
 H       2.472595     4.013454    -1.268813      17.08
 O       2.293664     3.567902     0.904228     318.53
 H       3.188665     3.504876     1.141830      29.95
 C       0.336663     3.449969    -0.385304      68.34
 H      -0.307401     3.111848    -1.247186      21.09
 C      -0.390536     4.776220    -0.101807      85.93
 O      -0.034793     6.081038    -0.854874     247.48
 H       0.210990     5.742235    -1.808682      27.61
 H      -0.101221     4.892957     0.975210      23.14
 H      -1.476468     4.576641    -0.475178      21.63
 C      -1.115731    -0.849938    -0.179119      46.23
 H      -0.567093    -1.824889    -0.547828      18.76
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 C      -3.141816     0.512215    -0.065685      62.03
 H      -4.096735     0.497795    -0.558153      14.89
 C      -2.273388     1.704746     0.253733       1.37
 O      -2.901427     2.876572     0.659420     187.48
 C      -4.168326     3.150892    -0.023835     116.91
 H      -4.810664     2.231442    -0.010552      24.54
 H      -4.406248     4.315266     0.273443      23.73
 H      -3.800933     3.269123    -1.007850      28.25
 C      -0.866394     1.590088     0.447440      28.36
 O      -0.054298     2.622641     0.714646     223.17
 C      -0.453036     0.295274     0.247330      48.91
 H       0.617287     0.007919     0.098646      19.72
 C      -2.543425    -0.827385    -0.318536       2.55
 C      -3.425730    -2.041170    -0.423428     102.04
 H      -4.126399    -1.835564    -1.186659      21.90
 O      -2.738961    -3.125215    -1.077740     284.84
 H      -3.269403    -3.869109    -0.847684      19.26
 C      -4.213890    -2.903576     0.735294      82.33
 H      -3.470911    -3.457560     1.304628      21.20
 O      -5.058218    -1.856701     1.498161     309.08
 H      -4.342764    -1.280975     2.115478      21.62
 C      -5.282024    -3.847569     0.280574      93.88
 O      -4.745988    -4.847238    -0.488015     354.80
 H      -4.090952    -5.203381     0.234139      27.46
 H      -5.940250    -3.280674    -0.293762      28.43
 H      -5.523776    -4.235858     1.292182      27.05
55
name = lig-etoh-frame_483
 C       2.315293     1.600065    -2.427881      47.85
 H       1.699397     2.453091    -2.853874      17.97
 C       3.215029     1.025643    -0.182120      52.40
 H       3.250347     1.009152     0.913075      17.48
 C       3.918516    -0.031844    -0.901767      14.04
 O       4.806408    -0.879003    -0.153534     252.87
 C       5.659636    -0.051531     0.793544      68.20
 H       6.363128     0.595805     0.129468      26.18
 H       6.184652    -0.654769     1.568733      26.29
 H       4.866186     0.562306     1.458424      26.18
 C       3.748998    -0.257149    -2.301166      26.29
 O       4.394799    -1.334492    -2.951830     165.42
 H       5.277080    -1.730202    -2.430135      22.06
 C       2.846085     0.523775    -3.002873      62.45
 H       2.804563     0.530617    -4.009667      28.54
 C       2.478954     1.930926    -0.986231      67.91
 C       1.913208     3.216154    -0.510081     103.57
 H       2.214738     4.174829    -1.048391      21.57
 O       2.323175     3.623427     0.942487     247.22
 H       3.395619     3.392282     0.776910      23.73
 C       0.311278     3.467203    -0.372435      74.69
 H      -0.219817     3.128077    -1.247192      21.51
 C      -0.345886     4.757845    -0.147172     110.31
 O      -0.017588     6.007272    -0.803958     278.72
 H       0.121207     5.828668    -1.800172      28.18
 H       0.081706     5.107359     0.786799      23.11
 H      -1.394032     4.517476    -0.234795      23.69
 C      -1.136598    -0.875377    -0.183850      43.44
 H      -0.688790    -1.733045    -0.613161      20.76
 C      -3.119701     0.519245    -0.099933      55.99
 H      -4.226037     0.570444    -0.304407      22.91
 C      -2.240318     1.653472     0.247202      17.52
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 O      -2.911774     2.880349     0.680370     197.46
 C      -4.187990     3.116221     0.041175     116.27
 H      -4.965476     2.356216     0.166556      25.90
 H      -4.532928     4.099273     0.392193      26.15
 H      -4.109395     3.227779    -1.147450      25.21
 C      -0.925388     1.615870     0.424293      26.07
 O      -0.042855     2.585513     0.699632     220.49
 C      -0.421755     0.257141     0.255533      24.07
 H       0.738813     0.034193     0.284108      19.65
 C      -2.569333    -0.716573    -0.187580      24.26
 C      -3.449464    -1.999559    -0.435285      67.17
 H      -4.449394    -1.875088    -1.108046      18.69
 O      -2.712466    -3.151147    -1.093566     233.69
 H      -3.243286    -3.994423    -0.993818      15.81
 C      -4.219883    -2.812566     0.737527      93.08
 H      -3.593874    -3.573280     1.324495      17.99
 O      -5.035072    -1.872205     1.505309     356.05
 H      -4.600183    -1.284272     2.243298      24.89
 C      -5.216163    -3.853017     0.294964      81.30
 O      -4.816022    -4.944235    -0.520875     326.94
 H      -4.133738    -5.547831    -0.077459      29.24
 H      -6.013846    -3.163276    -0.183041      26.49
 H      -5.558775    -4.136904     1.396610      26.29
55
name = lig-etoh-frame_484
 C       2.326054     1.686188    -2.411901      38.62
 H       1.742403     2.388525    -2.958376      21.44
 C       3.256550     1.051436    -0.166935      16.13
 H       3.638130     1.016687     0.893409      15.28
 C       3.865177    -0.004263    -0.889989       1.80
 O       4.784247    -0.820956    -0.118635     294.89
 C       5.667494    -0.061680     0.794461     115.26
 H       6.463749     0.420712     0.302027      28.00
 H       6.160796    -0.644855     1.570500      27.87
 H       5.190632     0.716908     1.288518      30.89
 C       3.822183    -0.354085    -2.339900       0.89
 O       4.392942    -1.332565    -2.955480     189.01
 H       5.081198    -1.560904    -2.151751      19.67
 C       2.769008     0.529442    -3.017378      55.93
 H       2.722608     0.459359    -4.205703      25.64
 C       2.498165     1.921497    -0.963980      47.16
 C       1.815708     3.281928    -0.446520      95.71
 H       2.140040     4.212838    -1.087414      22.59
 O       2.392768     3.648160     0.936776     255.51
 H       3.327362     3.612422     0.695454      27.62
 C       0.328522     3.412459    -0.427925      72.85
 H       0.052879     2.932489    -1.432684      21.02
 C      -0.285439     4.807084    -0.126825     109.47
 O       0.016246     5.937048    -0.797499     310.08
 H      -0.127788     5.958387    -1.743640      29.15
 H      -0.092683     5.161355     0.948214      23.45
 H      -1.410988     4.602242     0.113404      22.32
 C      -1.190154    -0.858291    -0.162073      46.72
 H      -0.726855    -1.818237    -0.485024      21.06
 C      -3.102417     0.562959    -0.122829      81.71
 H      -4.145458     0.786152     0.112428      24.32
 C      -2.353133     1.641161     0.255966       8.96
 O      -2.921324     2.867924     0.679339     215.33
 C      -4.201051     3.088519     0.057095     121.02
 H      -5.068062     2.465675     0.511606      25.09
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 H      -4.759372     4.033743     0.688103      24.47
 H      -4.367699     3.159372    -0.978135      27.81
 C      -0.931331     1.530097     0.393216      -1.89
 O      -0.036673     2.565726     0.718505     181.17
 C      -0.336613     0.202793     0.239893      29.53
 H       0.699937     0.248972     0.449679      18.70
 C      -2.585417    -0.700869    -0.090921      26.20
 C      -3.519511    -2.027189    -0.462657      70.94
 H      -4.378264    -1.612288    -0.946495      22.29
 O      -2.661442    -3.147324    -1.114848     203.24
 H      -3.324795    -4.021474    -1.254161      13.84
 C      -4.170325    -2.677745     0.776181     106.42
 H      -3.455274    -3.178336     1.447609      21.14
 O      -5.021858    -1.891529     1.515046     417.42
 H      -4.576741    -1.503488     2.213799      31.51
 C      -5.209710    -3.822843     0.335816      99.57
 O      -4.876029    -5.047526    -0.575071     279.59
 H      -4.301829    -5.700373    -0.211896      31.31
 H      -6.119146    -3.470715    -0.135699      28.05
 H      -5.741982    -4.186061     1.215534      26.71
55
name = lig-etoh-frame_485
 C       2.326287     1.770756    -2.326053      50.81
 H       1.727967     2.361356    -3.020785      20.92
 C       3.302338     1.063469    -0.205511      19.03
 H       3.644969     1.313293     0.761672      13.93
 C       3.860262    -0.017291    -0.890098       0.64
 O       4.768580    -0.762763    -0.084227     288.43
 C       5.683720    -0.077358     0.790337      94.17
 H       6.678606     0.258024     0.229397      25.52
 H       5.986829    -0.884903     1.520468      25.22
 H       5.414231     1.029591     1.251571      23.54
 C       3.754141    -0.314568    -2.316961       3.59
 O       4.432367    -1.366383    -2.942173     219.81
 H       5.017734    -1.704120    -2.248812      23.75
 C       2.778765     0.493312    -3.061340      49.10
 H       2.560791     0.303885    -4.075125      26.03
 C       2.481162     1.961708    -0.961948      56.99
 C       1.795416     3.381516    -0.354887      93.03
 H       2.172563     4.007437    -1.250078      24.15
 O       2.447915     3.665120     0.900401     244.84
 H       3.467737     3.865645     0.792713      26.78
 C       0.351304     3.336096    -0.476318      76.23
 H       0.143044     2.900278    -1.419709      22.12
 C      -0.275200     4.824776    -0.016121     102.16
 O       0.076039     5.917525    -0.837249     266.64
 H      -0.527723     5.941317    -1.727123      24.86
 H      -0.023069     4.914849     1.029923      25.77
 H      -1.362858     4.733252     0.101785      23.52
 C      -1.208338    -0.852110    -0.116557      50.16
 H      -0.846892    -1.928836    -0.160881      21.47
 C      -3.152417     0.616289    -0.097104      80.36
 H      -4.158848     0.772670     0.297817      23.84
 C      -2.411848     1.678607     0.285841       0.23
 O      -2.939442     2.851665     0.648838     209.79
 C      -4.293548     3.091743     0.163411     116.04
 H      -4.885340     2.347548     0.645750      26.57
 H      -4.549274     4.014857     0.618762      26.98
 H      -4.397232     3.120681    -0.999816      25.58
 C      -0.915908     1.403294     0.364666      -1.78
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 O      -0.063211     2.536392     0.739115     148.93
 C      -0.300628     0.194828     0.211578      41.00
 H       0.872549     0.274667     0.540377      15.67
 C      -2.601167    -0.788163    -0.071161      15.11
 C      -3.540732    -2.041912    -0.461546      64.33
 H      -4.308508    -1.454619    -1.162269      19.39
 O      -2.642199    -3.119202    -1.143046     264.96
 H      -3.268863    -3.724819    -1.351531      21.28
 C      -4.112957    -2.617005     0.803752      81.88
 H      -3.191449    -2.773744     1.475110      18.33
 O      -5.036908    -1.875537     1.531979     329.36
 H      -4.360090    -1.612288     2.395409      21.03
 C      -5.219705    -3.835729     0.363376      83.79
 O      -4.942071    -5.109555    -0.638411     210.93
 H      -4.363039    -5.714987    -0.022140      25.68
 H      -6.086936    -3.544358    -0.314243      25.39
 H      -5.760461    -4.406566     1.263174      24.84
55
name = lig-etoh-frame_486
 C       2.326072     1.754843    -2.297847      70.34
 H       1.601368     2.441221    -2.848114      16.94
 C       3.315986     1.105705    -0.290908      90.14
 H       3.527226     1.593384     0.723512      14.72
 C       3.896833    -0.029301    -0.878536      -9.33
 O       4.749706    -0.717712    -0.066167     271.97
 C       5.752982    -0.068642     0.781942     107.90
 H       6.625134    -0.096430     0.190527      27.20
 H       5.742750    -0.880006     1.504650      26.29
 H       5.497361     0.805866     1.180078      31.36
 C       3.635457    -0.251010    -2.282495      20.69
 O       4.460054    -1.386803    -2.920834     125.42
 H       5.196606    -2.060533    -2.326047      20.53
 C       2.822119     0.503282    -3.021575      59.23
 H       2.423367     0.193655    -4.049720      23.32
 C       2.451778     2.040298    -0.944891     103.90
 C       1.908357     3.418663    -0.331360     109.38
 H       2.204336     4.075834    -1.188521      28.33
 O       2.487245     3.692980     0.871139     283.91
 H       3.488497     4.053831     0.797328      27.39
 C       0.340280     3.316678    -0.422710      63.08
 H      -0.008083     2.923378    -1.429352      20.40
 C      -0.288682     4.786639     0.074624      91.42
 O       0.133697     5.921992    -0.894342     228.02
 H      -0.614297     5.808151    -1.468892      28.11
 H       0.339236     4.801194     1.038995      24.66
 H      -1.405178     4.754913    -0.039348      22.60
 C      -1.205129    -0.918202    -0.040647      48.22
 H      -0.868495    -1.908459     0.068051      22.62
 C      -3.240888     0.578439    -0.025856      73.36
 H      -4.346737     0.524469     0.166952      24.92
 C      -2.360608     1.676860     0.308551      -3.48
 O      -2.950614     2.868929     0.610957     185.98
 C      -4.389862     3.089148     0.281269      87.72
 H      -4.940803     2.199602     0.692912      23.85
 H      -4.353258     4.332110     0.526087      22.09
 H      -4.354788     3.011561    -0.804248      26.24
 C      -0.921560     1.381458     0.358425      12.26
 O      -0.119125     2.479891     0.739484     191.75
 C      -0.280480     0.189469     0.192571      55.09
 H       0.689760     0.017005     0.346188      19.59
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 C      -2.624913    -0.829763    -0.112898      18.28
 C      -3.504155    -1.992003    -0.479959      79.86
 H      -4.131925    -1.745915    -1.338702      19.94
 O      -2.644462    -3.045310    -1.159051     219.31
 H      -3.396847    -3.770168    -1.488297      15.83
 C      -4.089259    -2.647307     0.803505      82.68
 H      -3.123102    -2.714658     1.330278      19.29
 O      -5.032230    -1.819248     1.588308     359.41
 H      -4.600076    -1.539587     2.390493      28.17
 C      -5.236623    -3.918547     0.365976      77.94
 O      -4.987766    -5.141836    -0.669162     253.03
 H      -4.428450    -5.583678     0.022552      25.92
 H      -5.841175    -3.234050    -0.270719      26.92
 H      -5.528671    -4.336624     1.261022      25.78
55
name = lig-etoh-frame_487
 C       2.282401     1.704750    -2.330308      45.07
 H       1.612316     2.378183    -2.758306      19.59
 C       3.302052     1.206668    -0.344082      27.01
 H       3.545392     1.456917     0.663045      17.01
 C       3.922421     0.026817    -0.853832       7.00
 O       4.729386    -0.705693    -0.068061     245.75
 C       5.811839    -0.121176     0.758924      82.40
 H       6.783896    -0.302042     0.162211      23.64
 H       5.740054    -0.745092     1.713097      25.82
 H       5.483489     0.977339     1.211600      24.14
 C       3.630501    -0.309350    -2.207623      37.48
 O       4.461282    -1.394656    -2.895549     239.19
 H       5.056874    -1.779178    -2.368271      32.10
 C       2.811475     0.597550    -2.963016      70.41
 H       2.420389     0.217653    -3.935203      21.23
 C       2.460101     2.093159    -0.954525      39.55
 C       2.031048     3.382910    -0.411918      95.41
 H       2.186974     4.421754    -1.012273      20.68
 O       2.525613     3.745390     0.887010     306.27
 H       3.393302     3.969717     0.703028      30.40
 C       0.318902     3.355579    -0.304822      62.83
 H      -0.110207     3.048514    -1.247258      21.53
 C      -0.247069     4.723703     0.103414      97.20
 O       0.182406     5.901497    -0.909809     216.63
 H      -0.546047     5.842733    -1.550679      26.84
 H       0.315113     4.986808     0.953180      25.78
 H      -1.390228     4.728174     0.149946      23.10
 C      -1.210538    -0.991674     0.049213      14.88
 H      -0.709783    -2.047796     0.151896      17.42
 C      -3.285154     0.459437     0.066081      64.16
 H      -4.357010     0.417687    -0.105550      10.87
 C      -2.348907     1.590852     0.310477       5.11
 O      -2.937462     2.908373     0.585257     175.79
 C      -4.419138     3.104662     0.383396     114.26
 H      -5.188653     2.470933     0.873110      25.36
 H      -4.592728     4.058983     0.555449      28.29
 H      -4.541656     2.917003    -0.741045      24.82
 C      -0.941884     1.445720     0.368029      23.37
 O      -0.168200     2.429000     0.726045     229.56
 C      -0.352288     0.123738     0.168079      16.55
 H       0.836290    -0.227826     0.135421      14.26
 C      -2.634314    -0.770312    -0.177213      32.22
 C      -3.448026    -1.963302    -0.520167      82.69
 H      -4.253472    -1.834796    -1.354559      20.28
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 O      -2.665435    -2.977245    -1.176733     262.63
 H      -3.255503    -3.740232    -1.454291      22.82
 C      -4.102541    -2.700123     0.783138      56.56
 H      -3.210226    -3.049637     1.374948      22.27
 O      -5.020988    -1.768385     1.621393     330.54
 H      -4.648688    -1.404942     2.477600      26.72
 C      -5.206147    -3.973619     0.311926      76.14
 O      -5.019828    -5.125393    -0.650146     299.71
 H      -4.365918    -5.664582    -0.169419      29.85
 H      -5.830636    -3.125305     0.009153      27.37
 H      -5.524415    -4.278447     1.456577      25.35
55
name = lig-etoh-frame_488
 C       2.195627     1.700211    -2.347305      41.26
 H       1.512476     2.334767    -3.042227      21.21
 C       3.316790     1.290980    -0.325576      30.03
 H       3.639248     1.308942     0.743391      17.36
 C       3.916992     0.128396    -0.856211      35.78
 O       4.729117    -0.723621    -0.059656     285.63
 C       5.831673    -0.164343     0.763463     131.56
 H       6.787972    -0.122904     0.305232      28.27
 H       5.924666    -0.614263     1.720736      29.15
 H       5.760816     0.849482     0.865884      32.31
 C       3.699701    -0.404070    -2.141690      11.44
 O       4.395835    -1.351695    -2.875795     184.83
 H       5.196704    -1.569167    -2.064712      21.36
 C       2.801653     0.640021    -2.901439      60.99
 H       2.504666     0.388948    -3.907230      21.25
 C       2.511237     2.110742    -1.038833      26.32
 C       2.056014     3.399803    -0.484156      80.31
 H       2.177215     4.300911    -1.023041      18.79
 O       2.546769     3.789950     0.915393     240.17
 H       3.664956     3.823074     0.744276      21.78
 C       0.327873     3.407579    -0.196362      65.83
 H      -0.129997     3.136121    -1.179989      20.15
 C      -0.180266     4.718622     0.094889      99.64
 O       0.211737     5.844309    -0.887317     229.86
 H      -0.276453     5.936342    -1.845089      23.69
 H       0.157935     5.260966     1.072749      23.15
 H      -1.220843     4.665569     0.407995      23.81
 C      -1.226324    -1.051112     0.125933      51.35
 H      -0.803317    -1.975356     0.032591      19.44
 C      -3.262757     0.355998     0.141680      69.46
 H      -4.280404     0.552572    -0.292705      14.39
 C      -2.429787     1.504712     0.318578      -8.59
 O      -2.924496     2.928293     0.568813     170.92
 C      -4.411991     3.075187     0.434546     108.69
 H      -5.163678     2.692230     1.204109      25.47
 H      -4.883939     4.249217     0.728227      23.61
 H      -4.880567     2.861405    -0.569791      25.72
 C      -0.990571     1.424785     0.353631       5.83
 O      -0.168612     2.434707     0.733068     211.68
 C      -0.429034     0.034101     0.152022      26.89
 H       0.561969    -0.023160     0.053601      17.99
 C      -2.611007    -0.736988    -0.225170      31.91
 C      -3.453257    -1.979553    -0.560663      74.38
 H      -4.430116    -1.615222    -1.009642      21.95
 O      -2.654897    -2.927924    -1.206559     279.84
 H      -3.192784    -3.672659    -1.345988      23.18
 C      -4.115317    -2.745855     0.766732      62.69
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 H      -3.483936    -3.392558     1.439251      19.46
 O      -4.999239    -1.749029     1.613291     303.41
 H      -4.369964    -1.366180     2.471691      21.03
 C      -5.163392    -3.972549     0.313232     109.93
 O      -5.042337    -5.065099    -0.602923     314.62
 H      -4.282086    -5.736960    -0.423406      30.48
 H      -6.180748    -3.453643     0.057448      27.19
 H      -5.509749    -4.317523     1.192852      28.04
55
name = lig-etoh-frame_489
 C       2.091733     1.739813    -2.369011      37.58
 H       1.533040     2.196736    -3.086720      23.48
 C       3.377035     1.319265    -0.264811      34.61
 H       3.587304     1.500401     0.807724      17.35
 C       3.933801     0.181592    -0.862172      29.66
 O       4.749624    -0.749143    -0.035804     260.96
 C       5.839427    -0.178797     0.745730     103.33
 H       6.889512    -0.163092     0.211655      25.54
 H       6.005939    -0.683951     1.761061      26.29
 H       5.784284     1.029655     0.704050      26.98
 C       3.704376    -0.370239    -2.135766      19.76
 O       4.344453    -1.309029    -2.803636     233.79
 H       5.192334    -1.519423    -2.296807      26.59
 C       2.829905     0.557085    -2.849916      62.92
 H       2.689425     0.515376    -4.027693      19.56
 C       2.556740     2.154046    -1.118284      33.50
 C       1.989443     3.441336    -0.458332      71.44
 H       2.218084     4.259292    -1.396458      15.87
 O       2.594565     3.818861     0.908463     298.68
 H       3.517354     3.645043     1.011923      26.80
 C       0.392371     3.417360    -0.171002      68.40
 H      -0.038152     3.216796    -1.169487      19.97
 C      -0.125642     4.837474     0.121231     106.40
 O       0.229602     5.779928    -0.862862     315.71
 H       0.077146     5.666057    -1.785905      29.05
 H       0.210354     5.285217     1.033602      24.59
 H      -1.270009     4.592364     0.360884      22.16
 C      -1.286821    -1.092033     0.151365      54.49
 H      -0.909570    -2.149949    -0.152091      17.40
 C      -3.251546     0.360001     0.170224      77.82
 H      -4.206214     0.609598    -0.225751      16.97
 C      -2.498638     1.497511     0.359887      -3.60
 O      -2.943794     2.905607     0.545232     172.71
 C      -4.450594     3.095969     0.513592     115.85
 H      -4.713715     2.555421     1.467873      26.05
 H      -4.506265     4.071767     0.614544      28.30
 H      -4.980051     2.781123    -0.394271      26.83
 C      -1.069367     1.321697     0.322020      -3.84
 O      -0.146992     2.454837     0.765399     151.82
 C      -0.501164     0.048666     0.165932      31.52
 H       0.696109     0.158299     0.085633      14.89
 C      -2.574962    -0.852510    -0.231517      24.38
 C      -3.505131    -1.987616    -0.521746      74.63
 H      -4.458177    -1.515555    -0.927508      22.16
 O      -2.631671    -2.891741    -1.267971     191.85
 H      -3.234331    -3.824036    -1.253084      15.44
 C      -4.162711    -2.791124     0.751416      74.79
 H      -3.544552    -3.357678     1.433500      20.06
 O      -4.932796    -1.760400     1.588696     398.74
 H      -4.263305    -1.489764     2.098720      30.32
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 C      -5.188181    -3.913513     0.339306     107.60
 O      -5.041503    -5.001625    -0.587156     294.64
 H      -4.257405    -5.559796    -0.430773      31.13
 H      -6.188090    -3.789702    -0.071878      24.30
 H      -5.425836    -4.565361     1.377246      24.10
55
name = lig-etoh-frame_490
 C       2.084567     1.699931    -2.372544      96.07
 H       1.480535     2.300272    -3.082615      24.86
 C       3.426697     1.344495    -0.249653      51.40
 H       3.516814     1.755053     0.741541      17.81
 C       3.995061     0.166962    -0.803746       4.74
 O       4.771229    -0.764579    -0.016414     249.24
 C       5.881233    -0.133701     0.697056     103.59
 H       6.711508    -0.446766     0.105907      23.86
 H       5.888618    -0.667346     1.608266      27.60
 H       5.625992     0.869670     0.896415      29.62
 C       3.646787    -0.209681    -2.140850      10.29
 O       4.317760    -1.300042    -2.745125     170.79
 H       5.233647    -1.627267    -2.406809      23.95
 C       2.820037     0.484475    -2.857927      60.72
 H       2.914518     0.357292    -3.866732      21.15
 C       2.573924     2.216124    -1.114659      60.43
 C       1.932687     3.481684    -0.413194      92.09
 H       2.102572     4.142888    -1.176612      17.99
 O       2.586626     3.839870     0.878030     278.09
 H       3.617946     3.575318     0.942247      27.15
 C       0.472007     3.429000    -0.199010      52.04
 H       0.057066     3.230722    -1.200893      19.17
 C      -0.113466     4.933380     0.169135     107.50
 O       0.259360     5.748756    -0.841797     292.88
 H       0.186564     5.217125    -1.734260      26.37
 H       0.437348     5.263400     1.106241      23.19
 H      -1.176052     4.782205     0.103484      23.14
 C      -1.306670    -1.156823     0.109375      44.81
 H      -0.936163    -2.115882    -0.159987      18.59
 C      -3.245227     0.385662     0.137850      65.22
 H      -4.370245     0.459242    -0.033619      18.44
 C      -2.520084     1.565487     0.418979      10.83
 O      -2.969024     2.833412     0.499650     199.25
 C      -4.446286     3.082116     0.632375      87.05
 H      -4.519648     2.500669     1.532681      26.69
 H      -4.216615     4.324842     0.551178      21.63
 H      -5.029238     2.583153    -0.249155      24.79
 C      -1.124757     1.276856     0.317890       5.95
 O      -0.136855     2.445638     0.795044     100.02
 C      -0.502743     0.109767     0.200296      44.48
 H       0.557531     0.090770     0.248474      16.00
 C      -2.630196    -0.965225    -0.156829      19.22
 C      -3.564637    -2.017693    -0.445237      82.73
 H      -4.366888    -1.631737    -1.184284      20.32
 O      -2.650547    -2.894735    -1.342886     243.81
 H      -3.015763    -3.763767    -1.312671      20.94
 C      -4.240631    -2.811432     0.724949      78.14
 H      -3.312040    -3.160672     1.348186      19.56
 O      -4.858133    -1.810802     1.529013     367.10
 H      -3.994793    -1.348139     2.053356      20.64
 C      -5.277628    -3.905835     0.433255      95.64
 O      -4.997055    -4.948052    -0.613845     362.35
 H      -4.194530    -5.375381    -0.241254      28.60
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 H      -6.267557    -3.470069    -0.013518      25.11
 H      -5.253540    -4.357438     1.323941      26.82
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name = lig-etoh-frame_491
 C       2.156618     1.634447    -2.348930      82.16
 H       1.485304     2.331477    -2.895414      21.08
 C       3.449616     1.388570    -0.294737      64.18
 H       3.597344     1.836663     0.747210      14.01
 C       4.045788     0.146302    -0.701657      -0.29
 O       4.768783    -0.761419    -0.020949     299.23
 C       5.898091    -0.118369     0.650910      89.40
 H       6.770242    -0.374896    -0.023683      23.18
 H       5.877158    -0.720324     1.635646      27.10
 H       5.670318     0.952042     1.029963      28.41
 C       3.692658    -0.117131    -2.072671      31.86
 O       4.277999    -1.295357    -2.706201     105.43
 H       5.278296    -1.635258    -2.242163      19.05
 C       2.718730     0.519363    -2.915677      40.11
 H       2.932083     0.049226    -4.023055      25.35
 C       2.566253     2.224189    -1.072511      38.62
 C       1.941756     3.464360    -0.345347      97.34
 H       2.036037     4.545553    -1.057732      13.45
 O       2.551092     3.849084     0.849182     270.89
 H       3.546401     3.852397     0.542387      27.05
 C       0.465878     3.449432    -0.211621      46.75
 H       0.059392     3.195987    -1.224641      17.09
 C      -0.085917     4.935541     0.233677      97.64
 O       0.315731     5.765257    -0.871317     257.77
 H       0.161350     5.072661    -1.604176      25.57
 H       0.429409     5.208733     1.176914      23.58
 H      -1.266002     5.024791     0.176302      21.03
 C      -1.274341    -1.160215     0.031993      33.36
 H      -0.753564    -2.148918    -0.091960      18.01
 C      -3.265883     0.385129     0.078256      79.11
 H      -4.327206     0.270424     0.247184      24.58
 C      -2.522913     1.570677     0.441283       6.27
 O      -2.987143     2.772091     0.444602     224.74
 C      -4.377194     3.075575     0.734505     134.39
 H      -4.799725     2.713983     1.763898      27.07
 H      -4.502308     4.078641     0.680697      26.93
 H      -5.002204     2.615067     0.026249      28.83
 C      -1.121880     1.367616     0.362638       2.24
 O      -0.136205     2.418249     0.800613     124.20
 C      -0.514407     0.066807     0.241626      22.04
 H       0.609160    -0.004700     0.394862      16.58
 C      -2.734089    -0.965283    -0.009678      21.29
 C      -3.631348    -2.107021    -0.458670      79.03
 H      -4.297119    -1.793850    -1.250865      20.34
 O      -2.684812    -2.905895    -1.410123     235.19
 H      -2.963764    -3.847693    -1.421495      18.93
 C      -4.254092    -2.808696     0.692880     101.70
 H      -3.328133    -3.176486     1.091015      20.16
 O      -4.776433    -1.851244     1.492279     421.19
 H      -4.180495    -1.208375     1.993836      26.44
 C      -5.380388    -3.890268     0.481184      71.94
 O      -4.928881    -4.881431    -0.630839     337.79
 H      -4.168220    -5.300693    -0.045679      25.78
 H      -6.188946    -3.178309     0.377429      27.95
 H      -5.444150    -4.372772     1.624442      25.20
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name = lig-etoh-frame_492
 C       2.210646     1.652026    -2.309410      38.68
 H       1.484161     2.242818    -2.797211      19.35
 C       3.473751     1.449772    -0.304356      77.74
 H       3.759091     1.707170     0.667495      15.53
 C       4.018827     0.181883    -0.674919      19.83
 O       4.770425    -0.747516    -0.017495     330.66
 C       5.908500    -0.136341     0.648335     118.56
 H       6.823353     0.006971     0.043063      28.25
 H       6.146886    -0.716338     1.509073      29.79
 H       5.867259     0.951859     0.896398      30.46
 C       3.779382    -0.115232    -2.013616       9.14
 O       4.250927    -1.280221    -2.653271     215.52
 H       4.940241    -1.488946    -2.163533      25.31
 C       2.681725     0.526889    -2.969048      35.74
 H       2.490478     0.086856    -3.865718      26.36
 C       2.563353     2.164871    -1.025098      34.99
 C       1.961257     3.475535    -0.347097     112.97
 H       2.018573     4.359045    -0.885959      20.03
 O       2.526838     3.854689     0.834930     267.15
 H       3.422793     4.155133     0.614294      31.01
 C       0.368083     3.462423    -0.191501      59.23
 H      -0.021342     3.198978    -1.163636      18.76
 C      -0.073663     4.891387     0.266815     101.35
 O       0.382450     5.793635    -0.900339     294.58
 H       0.110175     5.403088    -1.717952      30.75
 H       0.347464     5.217089     1.217980      25.59
 H      -1.091311     5.020198     0.534464      25.13
 C      -1.264758    -1.102012    -0.039459      37.07
 H      -0.677934    -2.059117     0.013516      17.72
 C      -3.296547     0.343217     0.056882      60.60
 H      -4.365265     0.359445     0.367851      21.42
 C      -2.493884     1.469252     0.410816       2.00
 O      -3.024836     2.784200     0.408873     238.18
 C      -4.328582     3.030791     0.860952     126.56
 H      -4.793527     2.971674     1.824136      26.91
 H      -4.708425     4.223994     0.774303      24.38
 H      -5.131536     2.569361     0.096262      25.30
 C      -1.045714     1.468885     0.436165       1.31
 O      -0.143106     2.389372     0.786780     183.89
 C      -0.542842    -0.001122     0.283863       6.82
 H       0.588542    -0.048896     0.479843      16.29
 C      -2.778531    -0.930131     0.111418      13.93
 C      -3.661149    -2.196928    -0.568214      60.20
 H      -4.536869    -1.741528    -1.257385      19.24
 O      -2.724913    -2.923148    -1.458678     190.24
 H      -3.075404    -3.965966    -1.501989      14.67
 C      -4.208803    -2.853077     0.658828      99.72
 H      -3.354215    -3.540437     1.084633      17.01
 O      -4.750045    -1.851884     1.500052     404.28
 H      -4.199455    -1.274542     1.960872      29.78
 C      -5.426015    -3.869723     0.551994      86.78
 O      -4.871913    -4.791205    -0.597999     344.63
 H      -4.248629    -5.315056    -0.089763      31.59
 H      -6.367854    -3.174628     0.490075      27.42
 H      -5.743326    -4.401413     1.373356      28.37
55
name = lig-etoh-frame_493
 C       2.218406     1.710899    -2.293524      37.31
 H       1.350839     2.222882    -2.827864      17.65
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 C       3.528125     1.471081    -0.250792      68.50
 H       3.897563     1.771743     0.792776      14.92
 C       3.956243     0.248340    -0.732953      29.48
 O       4.792391    -0.721086     0.011125     315.24
 C       5.954635    -0.133691     0.650601     109.29
 H       6.795053     0.046232    -0.055058      28.29
 H       6.403386    -0.760449     1.489612      27.86
 H       5.729482     0.928674     0.927909      29.39
 C       3.780589    -0.148025    -2.070366      34.74
 O       4.217463    -1.253882    -2.601230     144.81
 H       5.061753    -1.684229    -1.876935      17.17
 C       2.739125     0.524984    -2.890690      50.99
 H       2.021028     0.152497    -3.844129      22.02
 C       2.551159     2.121506    -0.977539      49.73
 C       1.930510     3.444728    -0.391134      83.85
 H       2.106569     4.320747    -1.319635      19.68
 O       2.505905     3.858280     0.869723     250.06
 H       3.462116     4.339327     0.923345      27.78
 C       0.272583     3.460082    -0.152261      71.44
 H      -0.216650     3.245498    -1.150230      18.92
 C      -0.056820     4.850408     0.252240      85.32
 O       0.440502     5.819110    -0.889149     172.11
 H      -0.079224     5.839528    -1.847700      25.04
 H       0.622567     5.248503     1.123435      24.48
 H      -1.170446     4.904579     0.677511      22.97
 C      -1.324716    -1.040019    -0.062945      47.18
 H      -0.852202    -1.976124    -0.034772      19.13
 C      -3.338075     0.309125     0.103639      36.55
 H      -4.399403     0.611249     0.194505      19.99
 C      -2.434803     1.413964     0.356221     -12.02
 O      -3.052981     2.809697     0.395013     201.94
 C      -4.380189     3.034511     0.941039     117.28
 H      -4.418001     2.824341     2.125367      24.81
 H      -4.422364     4.054905     0.683129      26.10
 H      -5.076130     2.529315     0.379093      27.91
 C      -1.000814     1.425195     0.490592       9.71
 O      -0.130526     2.396879     0.779511     207.68
 C      -0.535740     0.037176     0.338378      27.58
 H       0.507315    -0.120206     0.461015      18.45
 C      -2.755639    -0.967840     0.108332      19.70
 C      -3.668482    -2.223258    -0.689539      63.85
 H      -4.544620    -1.777054    -1.099229      21.07
 O      -2.779306    -2.962335    -1.496279     274.80
 H      -3.221795    -3.756517    -1.522986      20.08
 C      -4.175249    -2.960802     0.672108     101.88
 H      -3.512187    -3.577147     1.160583      20.04
 O      -4.755265    -1.848144     1.525625     290.22
 H      -3.894881    -1.356909     2.069739      21.35
 C      -5.439092    -3.819698     0.566780      93.29
 O      -4.854792    -4.689656    -0.546789     318.72
 H      -4.263307    -5.385328    -0.110250      27.93
 H      -6.374019    -3.444760     0.129737      26.94
 H      -5.796522    -4.630824     1.400665      25.60
55
name = lig-etoh-frame_494
 C       2.204267     1.749724    -2.277313      28.07
 H       1.413565     2.230654    -2.778807      19.60
 C       3.581753     1.468499    -0.159557      55.41
 H       3.848848     1.879195     0.763918      14.92
 C       3.953876     0.278183    -0.795510      31.66
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 O       4.806019    -0.683579     0.036186     263.63
 C       6.022956    -0.095048     0.641968      91.96
 H       6.696934    -0.078731    -0.236777      29.12
 H       6.390530    -0.740017     1.443692      29.12
 H       5.555666     0.795362     1.202801      27.50
 C       3.688807    -0.145515    -2.157556      14.55
 O       4.243874    -1.295855    -2.543065     214.75
 H       4.857493    -1.717960    -1.995493      20.25
 C       2.776054     0.553914    -2.784171      61.70
 H       2.142449     0.221235    -3.500530      24.27
 C       2.523910     2.137765    -0.929092      75.92
 C       1.895453     3.422824    -0.475741      85.78
 H       2.076219     4.002586    -1.247635      26.45
 O       2.466145     3.868821     0.925458     290.28
 H       3.399523     4.105092     0.872743      31.70
 C       0.229908     3.427037    -0.163056      78.06
 H      -0.339445     3.298449    -1.063589      22.06
 C      -0.042861     4.870657     0.239368     108.68
 O       0.470595     5.839155    -0.866030     220.94
 H      -0.239053     6.048605    -1.496856      29.28
 H       0.750562     5.115873     0.863725      27.83
 H      -1.050201     4.913951     0.462409      27.07
 C      -1.409111    -0.984979    -0.027252      41.36
 H      -0.991901    -2.069481    -0.253608      18.98
 C      -3.339624     0.321082     0.189427      67.16
 H      -4.355755     0.619927    -0.082264      14.06
 C      -2.424696     1.446053     0.307090      -7.21
 O      -3.043590     2.797372     0.380784     189.25
 C      -4.396355     3.030028     1.044889      74.37
 H      -4.101576     2.711222     1.993091      26.90
 H      -4.371979     4.173264     0.714989      23.35
 H      -5.302508     2.322098     0.638151      22.90
 C      -1.008835     1.291430     0.512541      17.99
 O      -0.102818     2.433239     0.797680     195.75
 C      -0.505484     0.115004     0.383948      54.13
 H       0.637633    -0.207968     0.407748      18.37
 C      -2.754940    -1.037020    -0.024839      21.77
 C      -3.631146    -2.211128    -0.679780      53.91
 H      -4.646335    -1.741873    -1.167546      19.97
 O      -2.836487    -2.997124    -1.541364     227.03
 H      -3.459119    -3.866763    -1.608405      15.44
 C      -4.225532    -3.004501     0.711939      72.95
 H      -3.385806    -3.538532     1.338793      17.48
 O      -4.721926    -1.844379     1.567931     341.87
 H      -3.971704    -1.588430     2.064721      25.35
 C      -5.436423    -3.832675     0.533062      97.86
 O      -4.854029    -4.620681    -0.512448     344.55
 H      -4.277718    -5.359362    -0.110619      27.39
 H      -6.257490    -3.539207    -0.187271      25.17
 H      -5.601247    -4.430332     1.389303      27.01
55
name = lig-etoh-frame_495
 C       2.205349     1.772106    -2.192632      39.91
 H       1.440217     2.308278    -2.787967      17.52
 C       3.561182     1.458844    -0.142469      44.14
 H       3.840864     1.859368     0.872944      14.60
 C       4.033239     0.280329    -0.796245      38.26
 O       4.796254    -0.644170     0.036942     254.66
 C       6.041391    -0.055463     0.630016     108.09
 H       6.762243     0.097523    -0.183446      27.18
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 H       6.362661    -0.840883     1.361093      27.31
 H       5.834033     0.785499     1.259272      29.18
 C       3.658960    -0.166692    -2.110853       5.09
 O       4.252867    -1.369737    -2.543551     169.30
 H       4.973567    -1.702768    -1.799975      22.14
 C       2.726636     0.644112    -2.733363      72.48
 H       2.283349     0.045649    -3.712612      21.51
 C       2.521917     2.161800    -0.888783      72.37
 C       1.832653     3.373194    -0.469983      85.26
 H       2.095911     4.305127    -1.355367      21.24
 O       2.399338     3.870806     0.949380     243.65
 H       3.436929     3.812855     0.698616      25.70
 C       0.243100     3.389221    -0.228898      70.86
 H      -0.393968     3.211578    -1.148781      20.99
 C       0.005769     4.916195     0.191192      94.78
 O       0.475710     5.853735    -0.819712     237.03
 H      -0.338957     6.055140    -1.270145      29.13
 H       0.755269     5.042663     1.138837      25.34
 H      -1.140430     5.162575     0.387949      24.20
 C      -1.414166    -0.998512     0.025430      46.68
 H      -0.982920    -1.831137    -0.405425      19.98
 C      -3.297414     0.343395     0.244454      69.42
 H      -4.305073     0.452616    -0.235037      16.04
 C      -2.498510     1.499718     0.290419      15.35
 O      -3.010004     2.754599     0.349482     211.50
 C      -4.371122     2.999847     1.103110      93.10
 H      -4.041447     2.753470     2.188869      25.88
 H      -4.677853     4.096177     1.062082      25.68
 H      -5.216374     2.470588     0.945504      27.77
 C      -1.036530     1.307687     0.529245     -10.08
 O      -0.097337     2.448465     0.838880     176.66
 C      -0.443487     0.033573     0.388239      43.99
 H       0.556542    -0.068193     0.395506      17.54
 C      -2.818198    -1.023402    -0.201340      14.68
 C      -3.611524    -2.177963    -0.583034      81.25
 H      -4.408589    -1.817297    -1.158103      22.36
 O      -2.905403    -3.049081    -1.590390     242.17
 H      -3.547692    -3.858131    -1.710399      19.31
 C      -4.279197    -2.927729     0.785115      88.71
 H      -3.458863    -3.419507     1.232631      23.02
 O      -4.687121    -1.862525     1.605294     404.37
 H      -3.963891    -1.574506     2.238704      26.13
 C      -5.410909    -3.856387     0.445976      81.41
 O      -4.842552    -4.637326    -0.525913     398.79
 H      -4.227519    -5.229563    -0.111971      31.71
 H      -6.271554    -3.264688     0.062769      27.32
 H      -5.703707    -4.298230     1.537604      24.43
55
name = lig-etoh-frame_498
 C       2.145358     1.756641    -2.129836      40.40
 H       1.523635     2.538490    -2.705283      17.88
 C       3.452394     1.367210    -0.124172      22.93
 H       3.597268     1.593117     0.976604      21.07
 C       4.101069     0.326688    -0.740905      42.56
 O       4.924824    -0.514460     0.093211     262.41
 C       6.123378    -0.023930     0.608210      89.40
 H       6.672959     0.178884    -0.306862      22.28
 H       6.639383    -0.840293     1.279736      23.83
 H       5.699809     0.751070     1.409810      22.95
 C       3.641278    -0.234652    -1.967955      23.01
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 O       4.177240    -1.421201    -2.474989     184.38
 H       5.198571    -1.952044    -2.336462      23.85
 C       2.735212     0.562369    -2.697212      56.44
 H       2.560104     0.703682    -3.786859      21.41
 C       2.500569     2.230959    -0.819646      16.96
 C       1.819810     3.431981    -0.248300     107.71
 H       1.946740     4.060320    -1.027155      20.07
 O       2.221128     3.807233     0.951312     273.52
 H       3.308440     3.925389     1.012231      24.80
 C       0.283777     3.427248    -0.248534      53.32
 H      -0.090467     3.135882    -1.242434      17.19
 C      -0.104511     4.884355     0.202716     102.72
 O       0.507121     5.992854    -0.678731     208.44
 H       0.202976     5.806175    -1.625410      28.72
 H       0.539772     5.061286     0.971250      25.02
 H      -1.129591     4.808099     0.183213      24.72
 C      -1.249592    -1.143024    -0.081717      42.79
 H      -0.934966    -2.269212    -0.113313      16.86
 C      -3.347287     0.398243    -0.000505      50.00
 H      -4.348720     0.369551     0.414053      18.18
 C      -2.424554     1.469381     0.442261     -14.59
 O      -3.132271     2.821677     0.347359     244.87
 C      -4.133220     2.907170     1.343972     123.37
 H      -3.788654     2.558801     2.319386      26.92
 H      -4.413683     3.886759     1.095474      26.02
 H      -4.928792     2.109870     0.952444      25.36
 C      -1.061967     1.348668     0.530890      17.20
 O      -0.241549     2.426370     0.866620     199.19
 C      -0.598969     0.049511     0.365038      33.45
 H       0.520325    -0.218983     0.541124      16.13
 C      -2.613687    -0.872208    -0.305282      -1.07
 C      -3.680154    -2.062163    -0.567439      52.89
 H      -4.807036    -1.662524    -0.878925      18.96
 O      -3.099235    -3.100469    -1.570472     229.83
 H      -3.780455    -3.763544    -1.562052      15.98
 C      -4.097468    -2.773848     0.813483      71.05
 H      -3.319518    -3.351145     1.402964      17.84
 O      -4.749796    -1.772760     1.878681     290.90
 H      -3.875374    -1.321595     2.441518      18.93
 C      -5.370427    -3.685261     0.412479      82.11
 O      -4.883428    -4.866041    -0.663032     248.93
 H      -4.033094    -5.231783    -0.257199      23.48
 H      -6.079205    -3.375151    -0.361029      26.17
 H      -5.615740    -4.416369     1.196859      25.77
55
name = lig-etoh-frame_499
 C       2.170454     1.735581    -2.126532      31.13
 H       1.561274     2.166295    -2.859744      21.10
 C       3.402696     1.406888    -0.054329      30.23
 H       3.587599     1.658594     0.949869      21.43
 C       4.056891     0.286809    -0.726547      58.03
 O       4.957527    -0.532186     0.113700     259.12
 C       6.164619    -0.000887     0.631078     118.16
 H       6.884936     0.443402    -0.138340      24.51
 H       6.657488    -0.711185     1.205018      26.32
 H       6.003654     0.819240     1.262368      28.38
 C       3.665230    -0.242339    -2.013940      15.00
 O       4.123378    -1.412375    -2.458919     197.43
 H       5.015464    -1.611893    -2.229820      27.38
 C       2.772096     0.577714    -2.648083      58.40
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 H       2.549379     0.351026    -3.734539      20.24
 C       2.463120     2.155916    -0.845116      33.06
 C       1.857343     3.394533    -0.280426      93.28
 H       2.107251     4.216643    -1.244799      16.03
 O       2.230415     3.821247     1.090019     300.44
 H       3.122211     4.102859     0.946418      28.89
 C       0.284498     3.446739    -0.164397      75.57
 H      -0.133696     3.252998    -1.149522      18.63
 C      -0.205684     4.832807     0.174396      82.13
 O       0.498747     6.037006    -0.645881     151.09
 H       0.550004     5.637559    -1.628939      27.03
 H       0.438700     5.073929     1.135548      22.30
 H      -1.388530     4.862449     0.221305      22.12
 C      -1.253054    -1.092200    -0.151724      59.25
 H      -0.958911    -2.115273     0.073142      19.03
 C      -3.241712     0.444946    -0.061280      40.48
 H      -4.310235     0.246895     0.194564      19.43
 C      -2.503352     1.501251     0.429054      -7.80
 O      -3.108776     2.810191     0.381579     270.96
 C      -4.077813     2.843297     1.353473     125.36
 H      -3.632994     2.567487     2.321466      26.18
 H      -4.614695     3.996420     1.519111      24.22
 H      -5.038753     2.315646     1.355790      26.61
 C      -1.060673     1.308613     0.506016       5.62
 O      -0.293268     2.442702     0.837860     197.62
 C      -0.565795     0.032664     0.354187      40.33
 H       0.495259     0.056529     0.700427      16.60
 C      -2.648763    -0.965766    -0.286642      -0.33
 C      -3.664857    -1.982098    -0.619409      81.41
 H      -4.503852    -1.536170    -0.960614      22.44
 O      -3.183081    -3.044977    -1.500083     226.66
 H      -3.871445    -3.889704    -1.449964      10.43
 C      -4.080764    -2.774817     0.814436      67.24
 H      -3.217844    -3.246754     1.367677      17.76
 O      -4.772602    -1.752175     1.930265     299.99
 H      -4.055021    -1.291092     2.439107      21.67
 C      -5.279824    -3.691617     0.368039      76.55
 O      -4.903831    -4.897685    -0.682289     202.73
 H      -4.142911    -5.489668    -0.270572      24.18
 H      -6.088414    -3.294535    -0.331337      26.34
 H      -5.702505    -4.159263     1.332027      26.07
55
name = lig-etoh-frame_500
 C       2.203620     1.691533    -2.146537      74.61
 H       1.406749     2.027545    -2.896584      18.49
 C       3.356791     1.417496    -0.048613      16.89
 H       3.677555     1.740223     0.997518      15.71
 C       4.026302     0.241833    -0.637944      25.74
 O       4.960581    -0.561002     0.101929     267.37
 C       6.220273     0.067571     0.645134     108.27
 H       6.937471     0.466446    -0.010309      27.87
 H       6.739651    -0.841503     1.181484      25.56
 H       6.208149     1.056964     1.289867      25.70
 C       3.722729    -0.206566    -1.970103      15.40
 O       4.063552    -1.422575    -2.473352     112.37
 H       5.056108    -1.422328    -1.945974      20.29
 C       2.785186     0.593270    -2.671982      62.34
 H       2.476997    -0.132014    -3.539292      22.51
 C       2.445380     2.065253    -0.819470      67.06
 C       1.845973     3.395540    -0.324497     102.75
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 H       2.166087     4.207431    -0.829929      25.86
 O       2.264855     3.837089     1.201317     239.69
 H       3.165916     4.260622     1.068811      28.16
 C       0.274102     3.431477    -0.133557      81.59
 H      -0.201560     3.187836    -1.122540      20.34
 C      -0.263355     4.841615     0.188030     101.33
 O       0.465285     6.029592    -0.618754     239.85
 H       0.712018     5.705725    -1.437877      32.21
 H      -0.183699     5.053160     1.237233      25.98
 H      -1.296889     5.060050     0.192971      25.53
 C      -1.287613    -1.045252    -0.176241      55.47
 H      -0.754372    -2.009744     0.030449      19.06
 C      -3.143444     0.372709    -0.099376      32.99
 H      -4.257885     0.460394    -0.290281      21.67
 C      -2.560745     1.544786     0.352447      -1.13
 O      -3.057454     2.777464     0.402455     279.22
 C      -4.095945     2.843545     1.451516     126.17
 H      -3.534977     2.591836     2.376900      25.93
 H      -4.388260     3.776023     1.742767      26.72
 H      -5.062792     2.263381     1.422434      25.96
 C      -1.105614     1.334152     0.464980     -10.82
 O      -0.325272     2.468624     0.817613     209.54
 C      -0.474767     0.017187     0.349321      27.67
 H       0.558199     0.086153     0.696031      16.35
 C      -2.692238    -0.947688    -0.274904      32.54
 C      -3.629675    -1.970324    -0.611377      66.59
 H      -4.516504    -1.297586    -1.178065      17.88
 O      -3.264709    -2.982730    -1.440370     238.65
 H      -3.816938    -3.817205    -1.251516      13.02
 C      -4.118145    -2.706889     0.803059      82.23
 H      -3.225349    -3.187641     1.177760      20.09
 O      -4.797183    -1.780681     1.913558     300.66
 H      -4.066359    -1.254376     2.517676      20.19
 C      -5.179467    -3.758073     0.328596      92.30
 O      -4.918581    -4.910376    -0.671426     289.30
 H      -4.365119    -5.515206    -0.200450      29.45
 H      -5.941930    -3.053431    -0.051521      27.49
 H      -5.865996    -3.838453     1.260883      26.17
55
name = lig-etoh-frame_501
 C       2.184365     1.653072    -2.199091      39.73
 H       1.325411     2.158119    -2.585662      17.99
 C       3.375452     1.358725    -0.042546      24.92
 H       3.662764     1.801607     0.876664      15.38
 C       4.011547     0.213638    -0.528602      11.45
 O       4.973180    -0.569116     0.090480     255.37
 C       6.280703     0.129774     0.678503      88.74
 H       6.909548     0.289199    -0.307969      26.58
 H       6.664446    -0.709057     1.149281      28.67
 H       6.035759     0.914626     1.353821      28.97
 C       3.743240    -0.127020    -1.877392      28.10
 O       4.058697    -1.427060    -2.475798     186.94
 H       4.856385    -1.802884    -1.820121      19.07
 C       2.820920     0.507475    -2.720796      38.79
 H       2.336605    -0.063431    -3.445407      23.82
 C       2.408108     2.046721    -0.788411      92.65
 C       1.800562     3.384092    -0.265432      88.04
 H       2.295660     4.466116    -0.674884      22.94
 O       2.305274     3.839014     1.262408     190.16
 H       3.261752     4.306470     1.261642      27.46
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 C       0.232994     3.407603    -0.162615      80.20
 H      -0.155646     3.108735    -1.112159      20.61
 C      -0.293278     4.906039     0.208052      93.92
 O       0.414157     5.996240    -0.547384     223.46
 H       0.729627     5.665286    -1.446898      30.51
 H      -0.425192     5.070842     1.310148      24.91
 H      -1.403990     5.051741    -0.226813      23.04
 C      -1.269470    -1.024520    -0.130483      40.60
 H      -0.664007    -1.979265    -0.321989      19.06
 C      -3.167780     0.318724    -0.144809      59.11
 H      -4.055508     0.672402    -0.697254      22.05
 C      -2.495959     1.521868     0.244979       6.08
 O      -3.046995     2.769670     0.427992     241.05
 C      -4.109019     2.829013     1.592235      68.60
 H      -3.617876     2.349221     2.415983      26.09
 H      -4.171036     4.103866     1.729699      21.54
 H      -4.898183     2.110132     1.210813      24.20
 C      -1.140084     1.379622     0.422152       5.62
 O      -0.340418     2.496545     0.818094     212.47
 C      -0.441770     0.069823     0.329088      17.92
 H       0.716262    -0.150119     0.536868      17.73
 C      -2.645723    -0.872447    -0.272944      39.01
 C      -3.692449    -1.941805    -0.565665      94.12
 H      -4.439456    -1.441229    -1.023822      22.59
 O      -3.302961    -2.946832    -1.417090     281.39
 H      -3.774255    -3.765889    -1.180044      17.00
 C      -4.158699    -2.604875     0.784730      76.51
 H      -3.149531    -3.116472     1.088532      17.84
 O      -4.809055    -1.845094     1.844442     339.99
 H      -4.061563    -1.384941     2.452540      21.31
 C      -5.151668    -3.783393     0.320123      96.89
 O      -4.944651    -4.884125    -0.626448     319.51
 H      -4.419553    -5.562145    -0.027337      26.02
 H      -5.758855    -2.967798    -0.178985      27.14
 H      -5.764468    -4.096790     1.176940      26.76
55
name = lig-etoh-frame_502
 C       2.141523     1.630844    -2.179849      29.84
 H       1.308733     2.264506    -2.562209      17.56
 C       3.396604     1.315818    -0.020274      32.59
 H       3.658942     1.824620     0.936117      16.62
 C       4.025623     0.189208    -0.457105      17.61
 O       5.003961    -0.567715     0.106479     267.95
 C       6.297193     0.148719     0.654315      76.72
 H       6.779918     0.292033    -0.259852      27.89
 H       6.753224    -0.700239     1.312908      26.64
 H       5.884573     0.916382     1.333264      27.05
 C       3.741024    -0.124702    -1.829069      45.13
 O       4.081374    -1.421812    -2.436446     244.29
 H       4.632472    -2.059109    -1.966259      22.69
 C       2.831488     0.449895    -2.725971      30.73
 H       2.252216     0.039290    -3.698440      21.01
 C       2.384823     2.058967    -0.799633      68.67
 C       1.793192     3.413062    -0.142171      91.30
 H       2.091970     4.155364    -0.731963      25.54
 O       2.336750     3.823422     1.297629     283.21
 H       3.217342     4.097494     1.219090      30.77
 C       0.192925     3.421390    -0.184107      60.61
 H      -0.125511     3.127306    -1.235960      19.71
 C      -0.372096     4.963229     0.161394     109.47
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 O       0.376274     5.963090    -0.448919     240.07
 H       0.527239     5.577560    -1.413771      30.45
 H      -0.378180     5.125075     1.255777      25.65
 H      -1.182419     4.777964    -0.491014      24.16
 C      -1.179189    -1.010918    -0.058062      47.40
 H      -0.830623    -1.902226    -0.548050      17.75
 C      -3.257787     0.416044    -0.197948      85.12
 H      -4.090038     0.630819    -0.937884      17.12
 C      -2.419522     1.476408     0.148213       4.95
 O      -3.061374     2.771948     0.462036     215.44
 C      -4.074586     2.824920     1.676208      96.70
 H      -3.769681     2.101208     2.516811      26.18
 H      -4.195737     3.781966     1.676530      27.81
 H      -4.886667     2.315999     1.180299      26.62
 C      -1.067003     1.408484     0.398068      11.72
 O      -0.349601     2.521275     0.833726     221.59
 C      -0.452786     0.128837     0.280296      41.72
 H       0.528849    -0.111240     0.320377      17.73
 C      -2.582489    -0.874712    -0.296422       9.23
 C      -3.755291    -1.887282    -0.486266      61.13
 H      -4.797309    -1.369086    -0.929571      22.39
 O      -3.300171    -2.931848    -1.431218     228.74
 H      -3.748453    -3.922600    -1.211032      13.39
 C      -4.142114    -2.562830     0.771311      91.23
 H      -3.234887    -2.936342     1.172971      23.40
 O      -4.811989    -1.918210     1.752524     433.94
 H      -4.149398    -1.531438     2.286577      30.17
 C      -5.197963    -3.734861     0.328913      89.06
 O      -4.951364    -4.854244    -0.559434     271.22
 H      -4.398951    -5.521772    -0.061823      27.43
 H      -5.890776    -3.275539    -0.408703      26.17
 H      -5.574699    -4.465282     1.186362      22.91
55
name = lig-etoh-frame_503
 C       2.098798     1.619270    -2.097354      72.11
 H       1.465896     2.151754    -2.864284      20.43
 C       3.375595     1.345546     0.020845      71.02
 H       3.648308     1.704491     1.031726      17.61
 C       4.056179     0.168984    -0.457044      19.19
 O       5.056040    -0.578616     0.153824     302.74
 C       6.244030     0.108410     0.643311      89.84
 H       6.929856     0.549678    -0.194990      25.30
 H       6.846667    -0.493416     1.310574      28.36
 H       5.934054     1.103905     1.141626      29.00
 C       3.727138    -0.233731    -1.836391      31.27
 O       4.103437    -1.389276    -2.399187     106.14
 H       4.617292    -2.297466    -1.868949      16.91
 C       2.768089     0.474578    -2.697356      38.56
 H       2.641033     0.128679    -3.657597      21.88
 C       2.408705     2.055480    -0.796472      79.55
 C       1.785624     3.405009    -0.002493      95.88
 H       2.016339     4.153463    -1.011547      17.91
 O       2.333888     3.784153     1.290948     261.41
 H       3.373709     3.889501     1.067648      26.11
 C       0.198676     3.470240    -0.163551      72.91
 H      -0.067568     3.223250    -1.175723      19.50
 C      -0.451209     4.929393     0.083572     108.09
 O       0.368172     5.950360    -0.376307     279.59
 H       0.304238     5.778993    -1.282661      33.63
 H      -0.516678     5.125137     1.137520      26.43
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 H      -1.488668     4.759549    -0.435010      23.42
 C      -1.154994    -1.005067    -0.010650      49.87
 H      -0.775527    -1.959696    -0.565400      15.57
 C      -3.291942     0.501656    -0.290603      38.97
 H      -4.245221     0.557661    -0.770272      16.48
 C      -2.416973     1.510640     0.102272     -10.92
 O      -3.063317     2.763041     0.500433     220.22
 C      -4.011343     2.727305     1.669749      86.55
 H      -3.858811     2.124624     2.546625      26.26
 H      -4.291221     3.986946     1.933349      23.02
 H      -5.143057     2.601944     1.286756      23.53
 C      -0.955368     1.417348     0.385299       6.35
 O      -0.355550     2.546980     0.849207     212.96
 C      -0.461221     0.177098     0.216283      38.56
 H       0.775287     0.161522     0.182137      13.63
 C      -2.606836    -0.846997    -0.321090      -0.67
 C      -3.795924    -1.829737    -0.476031      80.54
 H      -4.661026    -1.383280    -0.721051      25.01
 O      -3.288847    -2.927647    -1.455173     252.77
 H      -3.690833    -3.714503    -1.299931      19.83
 C      -4.122074    -2.627630     0.740970      77.16
 H      -3.159411    -3.027033     1.298013      18.64
 O      -4.848857    -1.958836     1.679795     357.82
 H      -4.159058    -1.417945     2.413848      21.35
 C      -5.271734    -3.707987     0.352129      94.68
 O      -4.919385    -4.847579    -0.519704     340.67
 H      -4.269649    -5.426959    -0.101742      30.33
 H      -6.249901    -3.441850    -0.168805      26.18
 H      -5.528656    -4.119007     1.275309      26.34
55
name = lig-etoh-frame_504
 C       2.074412     1.597445    -2.054020      89.30
 H       1.579597     2.059381    -2.854364      23.49
 C       3.361810     1.358210     0.047316      53.56
 H       3.572079     1.600161     1.074873      17.99
 C       4.069258     0.174905    -0.518196      17.40
 O       5.108584    -0.602060     0.210686     304.14
 C       6.194034     0.130056     0.612773     126.63
 H       6.946436     0.545337    -0.059153      27.20
 H       6.843163    -0.445382     1.326662      26.32
 H       5.974994     1.067803     1.044302      30.36
 C       3.672271    -0.326646    -1.820168      10.90
 O       4.148570    -1.417937    -2.387379     220.89
 H       4.597310    -1.828592    -1.707497      28.55
 C       2.726324     0.520593    -2.580878      67.14
 H       2.946442     0.217335    -3.721879      20.13
 C       2.442492     2.061471    -0.715554      35.55
 C       1.766218     3.400922     0.013409     107.58
 H       2.055706     4.110011    -0.619861      19.44
 O       2.339032     3.738712     1.240523     283.45
 H       3.347172     3.723201     1.133831      27.83
 C       0.240929     3.533418    -0.095151      78.10
 H       0.019491     3.169143    -1.140613      21.03
 C      -0.552320     4.826042     0.031050     112.16
 O       0.365617     5.961154    -0.335844     221.64
 H       0.203389     6.197480    -1.349555      27.86
 H      -0.802339     5.006969     1.149578      24.69
 H      -1.593083     5.031228    -0.204187      24.35
 C      -1.229819    -1.012097    -0.028218      39.87
 H      -0.637258    -1.866315    -0.204989      15.94
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 C      -3.229706     0.520577    -0.393359      24.16
 H      -4.413690     0.641276    -0.349625      18.91
 C      -2.442536     1.604888     0.113395      -2.61
 O      -3.058673     2.750870     0.549895     254.46
 C      -4.017490     2.707502     1.612048     127.05
 H      -3.747947     2.041651     2.489759      25.97
 H      -3.936940     3.560853     2.132873      27.59
 H      -5.026925     2.585689     1.413304      26.40
 C      -0.965170     1.449338     0.361150     -11.41
 O      -0.352668     2.576861     0.865032     223.76
 C      -0.350735     0.189766     0.144396      22.56
 H       0.624399     0.314857     0.156539      15.39
 C      -2.683125    -0.765820    -0.333456      27.51
 C      -3.729013    -1.842017    -0.503289      54.36
 H      -4.758691    -1.229793    -0.822563      19.21
 O      -3.262932    -2.875062    -1.494631     188.50
 H      -3.909463    -3.760717    -1.296667      11.24
 C      -4.113057    -2.747705     0.712930     107.24
 H      -3.290817    -3.273200     1.083188      20.76
 O      -4.894121    -1.938476     1.670301     405.77
 H      -4.412317    -1.461165     2.262505      29.63
 C      -5.339992    -3.727294     0.379535      71.02
 O      -4.884679    -4.846492    -0.496140     283.30
 H      -4.019198    -5.254203     0.026211      24.07
 H      -6.322759    -3.253357     0.218685      28.96
 H      -5.597154    -3.776516     1.587783      24.41
55
name = lig-etoh-frame_505
 C       2.079046     1.597249    -2.000041      52.71
 H       1.417258     2.288869    -2.669237      19.76
 C       3.387230     1.311942     0.051826      57.91
 H       3.521534     1.554151     1.157035      17.30
 C       4.068185     0.185587    -0.577725      36.25
 O       5.104541    -0.630645     0.232085     248.58
 C       6.212120     0.192863     0.610720     105.70
 H       6.904407     0.331629    -0.309914      23.86
 H       6.693830    -0.482960     1.389626      24.96
 H       5.793055     1.116723     1.206651      27.43
 C       3.583040    -0.330091    -1.754756      15.91
 O       4.202855    -1.468617    -2.393563     171.37
 H       4.915142    -1.643805    -1.485535      19.01
 C       2.757916     0.494958    -2.476704      52.68
 H       2.806613     0.493819    -3.519774      16.55
 C       2.421352     2.087284    -0.619082      30.57
 C       1.767809     3.391001    -0.035979     102.48
 H       2.254953     4.419268    -0.621996      15.59
 O       2.348422     3.686398     1.215386     298.38
 H       3.283070     3.731973     1.215142      30.67
 C       0.254106     3.538122    -0.054555      83.47
 H       0.134856     3.081024    -1.031823      18.53
 C      -0.620569     4.786818     0.055168     107.78
 O       0.346979     5.975177    -0.319478     192.56
 H       0.062341     6.521644    -1.133090      29.34
 H      -0.790677     4.849023     1.102394      25.57
 H      -1.570290     4.958434    -0.507522      23.83
 C      -1.308404    -0.940702    -0.080323      21.83
 H      -0.742580    -1.940575     0.219432      14.65
 C      -3.168515     0.571832    -0.440200      52.52
 H      -4.129631     0.708194    -0.100213      19.60
 C      -2.441881     1.662577     0.138168      10.44
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 O      -3.051019     2.762362     0.585662     258.45
 C      -4.009017     2.673611     1.600062      73.76
 H      -3.640571     1.740139     2.129094      23.98
 H      -3.584308     3.595632     2.316877      21.21
 H      -5.145780     2.434599     1.283249      21.58
 C      -1.062670     1.490699     0.316510     -16.75
 O      -0.343063     2.599225     0.889626     215.41
 C      -0.323779     0.191671     0.076641      -4.86
 H       0.922199     0.151887     0.200655      10.63
 C      -2.709847    -0.722482    -0.337209      37.88
 C      -3.670964    -1.893788    -0.551583      91.91
 H      -4.499019    -1.447513    -0.922765      22.47
 O      -3.246714    -2.822144    -1.539218     271.46
 H      -3.924510    -3.503269    -1.463145      18.89
 C      -4.178566    -2.811938     0.673937      87.77
 H      -3.309241    -3.566451     0.985566      16.36
 O      -4.941216    -1.918667     1.656697     338.41
 H      -4.284409    -1.342156     2.322384      19.64
 C      -5.373321    -3.747225     0.476216      85.46
 O      -4.853925    -4.839021    -0.448039     366.17
 H      -4.096160    -5.073296     0.048413      33.86
 H      -6.201876    -3.043546     0.130832      28.20
 H      -5.575811    -4.046367     1.444380      28.60
55
name = lig-etoh-frame_506
 C       2.093398     1.660202    -1.884990       6.44
 H       1.424930     2.279138    -2.370219      19.13
 C       3.416918     1.261796     0.069281      36.48
 H       3.625775     1.461993     1.074484      17.99
 C       4.072373     0.188771    -0.542429      36.47
 O       5.039872    -0.642252     0.209153     241.51
 C       6.240162     0.245456     0.634933     111.30
 H       6.760381     0.235826    -0.321197      25.91
 H       6.684736    -0.391720     1.369324      27.10
 H       5.836038     1.072868     1.043426      33.61
 C       3.552928    -0.369231    -1.712587      21.18
 O       4.256423    -1.499748    -2.340325     200.53
 H       5.222533    -1.598864    -1.915705      23.20
 C       2.751967     0.495517    -2.427836      61.79
 H       2.544968     0.460984    -3.559756      18.37
 C       2.366363     2.088688    -0.580997      20.31
 C       1.848581     3.451034    -0.109172      99.58
 H       2.084943     4.171791    -0.762705      22.65
 O       2.343680     3.634096     1.234513     264.57
 H       3.404355     3.872931     1.179123      24.77
 C       0.243756     3.480523    -0.067323      73.14
 H       0.043201     3.063602    -1.071108      18.61
 C      -0.625504     4.821740     0.068362      96.27
 O       0.309581     5.992114    -0.291608     230.77
 H      -0.177231     6.495661    -0.886278      33.40
 H      -0.859620     4.878872     1.202954      23.66
 H      -1.283261     4.570504    -0.827557      22.15
 C      -1.306751    -0.850262    -0.116324      32.93
 H      -1.245666    -1.811164     0.329901      17.89
 C      -3.128736     0.652741    -0.417983      32.76
 H      -4.292113     0.728748    -0.185115      21.33
 C      -2.417858     1.664969     0.134903      20.26
 O      -3.034361     2.820367     0.578700     267.88
 C      -3.985908     2.602255     1.642959     113.47
 H      -3.813272     1.566978     1.954259      26.14
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 H      -3.923259     3.454729     2.195779      26.44
 H      -4.939529     2.622187     1.247245      26.98
 C      -1.076550     1.520722     0.271754      -3.36
 O      -0.339954     2.593624     0.922171     211.74
 C      -0.384878     0.215348     0.026136      31.30
 H       0.549299    -0.090615     0.248054      16.53
 C      -2.673348    -0.737826    -0.342180      19.78
 C      -3.636016    -1.963583    -0.572707      63.87
 H      -4.661278    -1.465877    -1.067560      18.93
 O      -3.204483    -2.774739    -1.613088     242.50
 H      -3.913910    -3.499704    -1.682444      18.21
 C      -4.249645    -2.819035     0.673493     106.50
 H      -3.456276    -3.370300     1.084442      19.59
 O      -4.946295    -1.891349     1.653997     370.00
 H      -4.152035    -1.442364     2.171401      22.30
 C      -5.376917    -3.755892     0.529043      89.88
 O      -4.863350    -4.809713    -0.400609     306.15
 H      -3.996364    -5.213865     0.098684      22.79
 H      -6.078194    -3.238531    -0.121859      26.49
 H      -5.695635    -4.558114     1.404179      23.64
55
name = lig-etoh-frame_507
 C       2.126121     1.696839    -1.767929      49.01
 H       1.367217     2.259219    -2.439108      19.41
 C       3.411182     1.256997     0.093851      27.82
 H       3.845715     1.465541     1.142383      17.36
 C       4.071430     0.148204    -0.443205      18.64
 O       4.965738    -0.619185     0.177072     245.45
 C       6.221819     0.229768     0.631556      95.28
 H       6.865128     0.408278    -0.253574      27.07
 H       6.881295    -0.317272     1.463693      25.02
 H       5.931533     1.360378     0.896045      27.95
 C       3.605526    -0.431733    -1.713842      -2.59
 O       4.288041    -1.499530    -2.288118     201.95
 H       5.299605    -1.682474    -2.126792      25.42
 C       2.683153     0.534971    -2.440891      52.36
 H       2.314028     0.114777    -3.412550      20.93
 C       2.369506     2.052013    -0.543048      39.20
 C       1.896409     3.466853    -0.124641      78.95
 H       2.108081     4.255410    -1.102197      21.06
 O       2.365457     3.612050     1.251882     282.43
 H       3.235755     3.986011     1.169221      26.05
 C       0.248956     3.424574    -0.096748      63.88
 H      -0.130701     3.116737    -1.089026      19.13
 C      -0.546557     4.846809     0.062829     111.45
 O       0.253515     5.997986    -0.252642     230.22
 H      -0.484362     6.499479    -0.798031      29.17
 H      -1.129720     4.994270     0.949632      26.58
 H      -1.193566     4.553890    -0.733423      24.61
 C      -1.313996    -0.807381    -0.137644      48.63
 H      -1.211538    -1.871326     0.271005      20.04
 C      -3.193316     0.641756    -0.358766      29.68
 H      -4.202806     0.776080    -0.625676      21.39
 C      -2.400929     1.697488     0.120182       1.14
 O      -3.003636     2.894144     0.555322     227.66
 C      -3.975820     2.514099     1.652289      90.53
 H      -4.055878     1.471128     2.180398      23.64
 H      -4.166059     3.427337     2.423730      23.47
 H      -5.013908     2.795325     1.102082      21.89
 C      -0.968491     1.532185     0.253432      13.99
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 O      -0.338246     2.556565     0.940110     227.27
 C      -0.528361     0.268713     0.004097      48.88
 H       0.534619    -0.118918     0.382052      17.03
 C      -2.665383    -0.713259    -0.370861      17.50
 C      -3.697298    -1.981358    -0.594214      69.81
 H      -4.536742    -1.478269    -0.876780      23.94
 O      -3.135639    -2.756561    -1.711384     229.81
 H      -3.780885    -3.604734    -1.895865      18.49
 C      -4.307020    -2.755909     0.737990      89.34
 H      -3.399317    -3.160466     1.383368      18.49
 O      -4.907871    -1.859743     1.644308     411.80
 H      -4.216140    -1.473954     2.114729      28.43
 C      -5.377220    -3.841038     0.519109     106.65
 O      -4.855789    -4.794661    -0.370825     372.20
 H      -4.157747    -5.383301    -0.011128      28.89
 H      -6.260790    -3.535957    -0.135032      26.18
 H      -5.857897    -4.310227     1.295613      26.13
55
name = lig-etoh-frame_508
 C       2.122145     1.658357    -1.806720      51.17
 H       1.452557     2.202242    -2.432831      21.13
 C       3.410031     1.277232     0.170414      21.24
 H       3.857996     1.614442     1.059521      17.77
 C       3.995224     0.092342    -0.409149      17.30
 O       4.968997    -0.585365     0.194281     266.87
 C       6.192137     0.220071     0.614928     115.06
 H       6.970712     0.414072    -0.193652      27.88
 H       6.728078    -0.176464     1.376473      28.84
 H       5.999816     1.222673     0.839023      31.32
 C       3.676016    -0.400570    -1.724905       3.09
 O       4.275443    -1.490843    -2.256860     149.77
 H       5.390906    -1.787800    -2.030172      20.05
 C       2.631104     0.500135    -2.424984      66.70
 H       2.131546     0.017503    -3.257389      22.77
 C       2.447744     2.038833    -0.441550      52.66
 C       1.886446     3.435218    -0.126427     107.16
 H       2.239959     4.163376    -0.760385      26.62
 O       2.383022     3.629257     1.247223     280.75
 H       3.257117     4.097983     1.257231      26.68
 C       0.278972     3.428861    -0.100979      73.85
 H      -0.086874     3.088258    -1.040686      22.49
 C      -0.453444     4.820505     0.046670     118.95
 O       0.183361     6.023610    -0.224798     230.97
 H      -0.472477     6.572466    -0.752692      30.53
 H      -1.282388     4.983499     0.847943      24.06
 H      -1.373749     4.882158    -0.713394      23.61
 C      -1.375069    -0.873255    -0.150009      54.34
 H      -0.679725    -1.748366    -0.030028      18.30
 C      -3.269980     0.589556    -0.307786      73.97
 H      -4.195138     0.888254    -0.958607      17.38
 C      -2.376026     1.737736     0.094075     -14.51
 O      -2.972975     2.942550     0.560013     199.39
 C      -4.052845     2.496638     1.637391      82.56
 H      -4.038645     1.592283     2.162136      28.89
 H      -3.975874     3.159898     2.495509      26.86
 H      -4.917115     2.566279     1.098051      25.84
 C      -0.942185     1.564163     0.260181       3.89
 O      -0.303174     2.516412     0.936064     231.41
 C      -0.559012     0.290221     0.035140      35.25
 H       0.468207     0.214935     0.400123      17.49
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 C      -2.733808    -0.679119    -0.413092      27.92
 C      -3.744116    -1.962027    -0.601361      39.94
 H      -4.763180    -1.357929    -0.929609      23.55
 O      -3.073814    -2.757028    -1.808277     250.14
 H      -3.541459    -3.511298    -1.907969      25.07
 C      -4.310539    -2.701200     0.835470      85.09
 H      -3.485818    -3.111891     1.357272      22.43
 O      -4.887962    -1.801466     1.630145     344.68
 H      -4.161832    -1.269384     2.329048      20.57
 C      -5.391039    -3.909217     0.452718      83.37
 O      -4.839711    -4.824828    -0.387262     359.09
 H      -4.216681    -5.426707     0.092716      27.16
 H      -6.343769    -3.545691     0.054397      28.00
 H      -5.938865    -4.055785     1.623592      24.88
55
name = lig-etoh-frame_509
 C       2.125696     1.578975    -1.852479      15.34
 H       1.414790     2.238970    -2.422031      17.45
 C       3.429948     1.280371     0.258626      37.63
 H       3.845421     1.767385     1.189355      14.78
 C       3.886806     0.071898    -0.420785      18.54
 O       5.042768    -0.563968     0.256934     276.50
 C       6.160096     0.218492     0.556534      83.03
 H       6.898918     0.158472    -0.236075      27.07
 H       6.570175    -0.336362     1.589660      23.99
 H       5.810524     1.253121     0.934856      25.60
 C       3.706680    -0.287277    -1.723149      22.07
 O       4.265390    -1.496568    -2.246951     208.12
 H       5.060576    -1.705234    -1.784352      20.74
 C       2.621405     0.393484    -2.374001      55.66
 H       1.990680     0.080916    -3.309030      23.48
 C       2.507144     2.044089    -0.443737      52.07
 C       1.869835     3.353902    -0.043982     109.17
 H       2.411616     4.298339    -0.673068      22.48
 O       2.388261     3.674510     1.251871     246.44
 H       3.324460     4.189290     1.291069      25.76
 C       0.325134     3.478591    -0.087228      70.21
 H       0.089373     2.992697    -1.089950      19.22
 C      -0.482539     4.785684     0.012308     117.60
 O       0.154775     6.090517    -0.196801     264.96
 H      -0.341164     6.581712    -0.781731      34.65
 H      -0.891627     4.719061     1.039341      24.99
 H      -1.208099     4.863939    -0.716987      25.87
 C      -1.377700    -0.924059    -0.160270      34.22
 H      -0.606261    -1.644514    -0.456350      18.00
 C      -3.315249     0.612126    -0.288400      67.14
 H      -4.152071     0.914159    -0.883566      17.73
 C      -2.386024     1.752094     0.066075      -0.34
 O      -2.959180     2.950121     0.592935     195.88
 C      -4.110331     2.517754     1.604040      30.60
 H      -3.736709     1.399788     1.934739      22.84
 H      -3.868494     3.223088     2.438115      23.94
 H      -5.164963     2.391021     1.056828      22.62
 C      -1.064644     1.591511     0.271320       2.36
 O      -0.218330     2.509520     0.922484     193.79
 C      -0.536308     0.258105     0.092376       9.99
 H       0.581786     0.261174     0.342613      15.16
 C      -2.834745    -0.727846    -0.442998      18.74
 C      -3.786488    -1.885984    -0.629256      56.19
 H      -4.694493    -1.622230    -1.078406      24.54
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 O      -3.025574    -2.730566    -1.868075     163.34
 H      -3.517957    -3.672897    -1.850775      18.86
 C      -4.284210    -2.697671     0.852899      59.93
 H      -3.378634    -3.303858     1.272237      18.35
 O      -4.887236    -1.683778     1.657638     366.73
 H      -4.315262    -1.303134     2.274767      27.91
 C      -5.429190    -3.887118     0.475634      90.16
 O      -4.825548    -4.896283    -0.422844     334.63
 H      -4.146396    -5.359440     0.265090      24.19
 H      -6.308863    -3.357031     0.014403      29.15
 H      -5.538794    -4.137030     1.439714      29.50
55
name = lig-etoh-frame_510
 C       2.141645     1.521709    -1.826193      36.25
 H       1.386273     2.124079    -2.398652      18.58
 C       3.438049     1.280094     0.312363      30.94
 H       3.783208     1.628159     1.295837      15.83
 C       3.877093     0.099754    -0.348966       9.44
 O       5.064278    -0.573902     0.300140     262.99
 C       6.144787     0.214123     0.566039     110.46
 H       6.895301     0.033409    -0.259781      26.89
 H       6.456216    -0.253618     1.390003      28.45
 H       5.828215     1.240010     0.813731      29.85
 C       3.696422    -0.227272    -1.744199       7.42
 O       4.231597    -1.470584    -2.253124     145.88
 H       4.906416    -1.720611    -1.287894      14.92
 C       2.591399     0.295079    -2.357331      63.79
 H       2.236917     0.049945    -3.291375      25.05
 C       2.526366     2.031595    -0.551251      32.98
 C       1.915726     3.342759     0.043853     113.43
 H       2.210161     4.057243    -0.684510      22.85
 O       2.393112     3.735972     1.301377     303.41
 H       3.230484     4.098964     1.152441      29.75
 C       0.389379     3.492973    -0.110172      72.19
 H       0.261383     3.041237    -1.056398      20.86
 C      -0.515454     4.775942     0.008971      90.04
 O       0.160053     6.159476    -0.150353     210.01
 H      -0.296717     6.540463    -1.015563      29.57
 H      -0.563363     4.604754     1.129925      22.12
 H      -1.337585     4.535988    -0.818695      21.49
 C      -1.343253    -0.904902    -0.187501      17.34
 H      -0.998665    -1.840628    -0.774757      15.97
 C      -3.301695     0.650709    -0.298934      41.53
 H      -4.379926     0.923431    -0.616046      17.51
 C      -2.487508     1.759937     0.055812       7.90
 O      -2.980291     2.933522     0.626787     218.33
 C      -4.116816     2.501721     1.540006      76.61
 H      -3.721124     1.622659     1.723058      28.24
 H      -4.099224     3.397960     2.298947      23.85
 H      -5.130270     2.441263     1.256243      24.76
 C      -1.139989     1.555987     0.307199       0.61
 O      -0.137380     2.515393     0.893228     129.04
 C      -0.547053     0.216421     0.158960      24.92
 H       0.602440     0.048206     0.141119      15.69
 C      -2.884466    -0.760494    -0.437120      17.44
 C      -3.793768    -1.855449    -0.676258      52.83
 H      -4.793332    -1.729831    -1.274238      20.28
 O      -3.012251    -2.707099    -1.887194     146.45
 H      -3.404495    -3.658790    -1.703417      18.79
 C      -4.253430    -2.704036     0.793860      63.07
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 H      -3.403845    -3.252757     1.193253      18.32
 O      -4.901660    -1.588259     1.666486     288.03
 H      -4.156208    -1.231720     2.415343      19.73
 C      -5.402806    -3.797610     0.487340      76.28
 O      -4.821842    -4.958813    -0.429109     294.14
 H      -4.092476    -5.290267     0.075799      26.65
 H      -6.226487    -3.334549    -0.037069      27.38
 H      -5.466710    -4.534555     1.503361      24.78
55
name = lig-etoh-frame_511
 C       2.135842     1.486805    -1.785637      67.17
 H       1.397967     1.952751    -2.383072      20.92
 C       3.408192     1.272067     0.291735      40.09
 H       3.665868     1.445628     1.334804      17.43
 C       3.968004     0.143232    -0.248318       3.14
 O       4.988430    -0.619426     0.306823     280.57
 C       6.171365     0.221756     0.570650      86.63
 H       6.922205     0.170714    -0.202280      27.18
 H       6.744181    -0.192134     1.600156      24.83
 H       5.999766     1.315741     0.612532      29.40
 C       3.677392    -0.267106    -1.727810       0.32
 O       4.211948    -1.415442    -2.201484     244.79
 H       4.622236    -1.755241    -1.527181      23.46
 C       2.554054     0.260498    -2.358445      64.19
 H       2.482086    -0.139598    -3.487976      23.32
 C       2.542188     2.009685    -0.606998      43.02
 C       1.956202     3.358110     0.077332      86.45
 H       2.226663     4.165682    -0.886072      19.15
 O       2.397396     3.796806     1.361947     256.04
 H       3.389885     4.064225     1.150756      25.39
 C       0.464929     3.461255    -0.145641      66.95
 H       0.294765     3.081503    -1.203625      19.40
 C      -0.491038     4.771733     0.021281      95.01
 O       0.138114     6.204865    -0.124346     240.06
 H      -0.035294     6.336188    -1.122143      29.71
 H      -0.747032     4.826161     1.101891      24.74
 H      -1.396317     4.485592    -0.444562      25.79
 C      -1.386844    -0.888607    -0.263629      35.19
 H      -1.288241    -1.863627    -0.646034      18.56
 C      -3.321319     0.646302    -0.347276      37.48
 H      -4.405595     0.785599    -0.109217      19.74
 C      -2.571189     1.761089     0.075914      -5.16
 O      -3.042209     2.919436     0.637276     241.37
 C      -4.101122     2.551707     1.488305      84.30
 H      -3.826024     1.440458     2.076200      20.87
 H      -4.265983     3.312666     2.198788      25.50
 H      -5.213302     2.496923     1.086003      23.25
 C      -1.107745     1.479350     0.369508      -8.26
 O      -0.106870     2.500611     0.844579     130.39
 C      -0.582982     0.171176     0.194316      43.76
 H       0.443738    -0.029707     0.090692      18.07
 C      -2.844411    -0.679268    -0.395480      12.86
 C      -3.805608    -1.900463    -0.747658      60.23
 H      -4.753295    -1.578360    -1.238704      21.13
 O      -3.027484    -2.692386    -1.855129     231.95
 H      -3.284154    -3.545761    -1.667211      22.15
 C      -4.261772    -2.667203     0.696347      76.36
 H      -3.341411    -3.069519     1.228080      19.12
 O      -4.885277    -1.529341     1.656493     300.67
 H      -4.126303    -1.300006     2.322199      20.96
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 C      -5.296056    -3.759619     0.518464     103.26
 O      -4.840806    -4.973806    -0.438995     258.65
 H      -3.925003    -5.347388    -0.031292      24.73
 H      -6.249899    -3.437710     0.018864      26.85
 H      -5.767443    -4.362302     1.223857      26.57
55
name = lig-etoh-frame_512
 C       2.093562     1.451425    -1.801584      79.88
 H       1.275059     2.006942    -2.435243      19.80
 C       3.374426     1.254165     0.245683      22.59
 H       3.467819     1.481120     1.357953      18.77
 C       4.063966     0.156458    -0.252126      31.34
 O       4.922821    -0.658114     0.327522     263.36
 C       6.240773     0.212564     0.610309      77.91
 H       6.946383     0.095764    -0.268539      24.33
 H       6.731996     0.039726     1.457145      27.78
 H       5.994093     1.331138     0.524788      27.89
 C       3.632087    -0.317957    -1.615434      18.32
 O       4.189188    -1.363840    -2.176225     144.33
 H       4.821027    -2.024388    -1.481763      19.69
 C       2.570825     0.241987    -2.379575      46.00
 H       2.463266    -0.087989    -3.333228      26.63
 C       2.555166     2.018684    -0.545465      58.85
 C       1.998201     3.417137     0.003950     102.47
 H       2.385753     4.178795    -0.586912      20.63
 O       2.423362     3.857569     1.385177     284.42
 H       3.454928     3.967670     1.462427      26.55
 C       0.494342     3.420537    -0.179804      69.36
 H       0.298303     3.169588    -1.201424      21.19
 C      -0.410820     4.787772     0.098725      94.38
 O       0.094054     6.203632    -0.138578     257.32
 H       0.265551     6.240934    -1.065489      32.72
 H      -0.882338     4.962774     1.094210      24.22
 H      -1.501372     4.697895    -0.357571      22.82
 C      -1.519594    -0.872699    -0.342248      59.27
 H      -1.084465    -1.973718    -0.377846      19.11
 C      -3.386206     0.647175    -0.347958      53.53
 H      -4.380303     0.601212     0.059333      18.86
 C      -2.532405     1.722040     0.120832     -22.51
 O      -3.112195     2.907633     0.627351     244.70
 C      -4.144815     2.564276     1.495022     109.89
 H      -4.149547     1.854845     2.184321      27.98
 H      -4.317284     3.441413     2.305574      24.12
 H      -4.940746     2.438183     0.764157      24.47
 C      -1.066175     1.433510     0.420382      -3.05
 O      -0.124001     2.451479     0.786518     171.81
 C      -0.634092     0.123944     0.192549      22.62
 H       0.583796    -0.012082     0.223659      16.83
 C      -2.786001    -0.599618    -0.378451      16.77
 C      -3.785672    -1.928875    -0.796482      66.22
 H      -4.725381    -1.406093    -1.197604      22.07
 O      -3.067012    -2.666966    -1.782102     215.51
 H      -3.278579    -3.735745    -1.665225      15.73
 C      -4.259991    -2.586630     0.612557      89.48
 H      -3.331239    -2.813550     1.187991      20.05
 O      -4.855457    -1.517962     1.596438     337.70
 H      -4.136112    -1.279726     2.257473      23.06
 C      -5.217903    -3.772461     0.485330      94.68
 O      -4.847156    -4.948882    -0.440993     288.84
 H      -4.042127    -5.368669    -0.039363      27.60
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 H      -6.099806    -3.399407    -0.034729      26.26
 H      -5.860932    -4.129919     1.506995      24.69
55
name = lig-etoh-frame_513
 C       2.030571     1.451900    -1.839209      64.12
 H       1.362747     2.013613    -2.357184      24.60
 C       3.365905     1.235396     0.249863      28.21
 H       3.412413     1.603704     1.229638      18.95
 C       4.076246     0.153970    -0.357093      42.85
 O       4.934842    -0.684648     0.395392     247.47
 C       6.283957     0.211307     0.587002      73.01
 H       6.853157    -0.176637    -0.240864      23.42
 H       6.750427    -0.022856     1.694250      24.23
 H       5.884926     1.183881     0.587921      29.59
 C       3.575834    -0.346018    -1.463529      32.45
 O       4.193455    -1.378141    -2.158387     224.40
 H       5.036697    -1.869241    -1.716029      25.46
 C       2.622855     0.273462    -2.330469      33.15
 H       2.248107    -0.082699    -3.399234      17.60
 C       2.519058     2.045554    -0.501250      30.72
 C       2.060327     3.462473    -0.049067      75.48
 H       2.637593     4.409277    -0.643482      17.94
 O       2.441858     3.897921     1.393050     314.27
 H       3.366694     3.909185     1.526888      28.40
 C       0.460120     3.424711    -0.174565      60.34
 H       0.259626     3.193966    -1.244339      19.76
 C      -0.364817     4.828707     0.185465      96.52
 O       0.055952     6.173873    -0.164266     224.20
 H       0.556052     6.163696    -1.097229      29.96
 H      -0.644747     4.838916     1.304869      23.11
 H      -1.179166     4.843182    -0.526250      22.95
 C      -1.511811    -0.892519    -0.365779      66.82
 H      -1.030043    -1.779430    -0.199288      21.24
 C      -3.418894     0.687257    -0.279701      42.40
 H      -4.557329     0.549604    -0.050412      18.48
 C      -2.461267     1.661387     0.190370     -10.28
 O      -3.122834     2.886974     0.607938     222.10
 C      -4.264282     2.643064     1.519593      99.46
 H      -4.186319     1.705299     2.374347      23.25
 H      -4.389060     3.558893     1.993582      25.51
 H      -5.048949     2.399620     0.753324      24.13
 C      -1.061006     1.424825     0.422135      12.90
 O      -0.153366     2.388211     0.734259     196.79
 C      -0.638769     0.086520     0.165729      27.65
 H       0.319924    -0.050555     0.398082      18.98
 C      -2.864423    -0.606006    -0.437697       5.38
 C      -3.767239    -1.873305    -0.787940      78.57
 H      -4.668962    -1.349866    -1.272014      22.19
 O      -3.113525    -2.680077    -1.700549     282.87
 H      -3.374380    -3.620498    -1.664132      19.63
 C      -4.215380    -2.485063     0.563424      91.16
 H      -3.265143    -2.785894     1.040444      20.66
 O      -4.832333    -1.537599     1.484396     349.65
 H      -4.105023    -1.207862     2.268551      20.98
 C      -5.212858    -3.811613     0.443297      88.98
 O      -4.848058    -4.892658    -0.421044     344.30
 H      -4.161758    -5.416921     0.079281      27.43
 H      -5.976622    -3.278704    -0.186476      27.01
 H      -5.335710    -3.792044     1.499605      27.36
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name = lig-etoh-frame_514
 C       2.015910     1.484192    -1.815351      56.90
 H       1.291737     2.108748    -2.529193      20.45
 C       3.360346     1.250013     0.252181      21.66
 H       3.686614     1.660262     1.300658      16.99
 C       4.065620     0.156011    -0.344944      29.52
 O       4.987359    -0.676617     0.473751     256.95
 C       6.284262     0.150979     0.592972      88.97
 H       6.905468    -0.267621    -0.197741      25.67
 H       6.604186    -0.172650     1.553568      26.96
 H       5.909272     1.258168     0.576028      27.80
 C       3.527523    -0.426486    -1.460428      22.85
 O       4.203175    -1.416603    -2.155627     214.41
 H       5.179206    -1.635840    -1.815762      23.90
 C       2.634768     0.346674    -2.263917      50.75
 H       2.228417    -0.123038    -3.125512      20.48
 C       2.460929     2.053969    -0.522482      21.47
 C       2.120086     3.512658    -0.062110      77.27
 H       2.533156     4.220168    -0.758083      20.90
 O       2.422824     3.914134     1.380172     282.79
 H       3.517436     3.917058     1.374656      23.52
 C       0.418483     3.485903    -0.152181      52.29
 H       0.192533     3.236377    -1.195169      19.49
 C      -0.329506     4.844084     0.248793     102.96
 O       0.068203     6.156615    -0.192131     269.30
 H       0.610337     6.022540    -0.994434      32.11
 H      -0.378618     4.721628     1.310791      23.87
 H      -1.183266     4.630455    -0.494025      21.48
 C      -1.446428    -0.889505    -0.332789      28.91
 H      -1.100364    -2.018932    -0.267956      20.16
 C      -3.413510     0.676813    -0.180098      27.13
 H      -4.452767     0.872317    -0.294293      20.77
 C      -2.465516     1.631736     0.280089       2.97
 O      -3.091928     2.854530     0.601663     175.71
 C      -4.390108     2.689943     1.530111      93.12
 H      -4.100129     1.967496     2.138325      28.63
 H      -4.563981     3.856047     1.749825      23.30
 H      -5.392019     2.377545     1.070815      25.41
 C      -1.090218     1.407145     0.361367      29.33
 O      -0.155598     2.352436     0.703846     180.22
 C      -0.655713     0.091070     0.128127      35.67
 H       0.433255    -0.280243     0.602727      17.09
 C      -2.976970    -0.649284    -0.543551      -4.84
 C      -3.788352    -1.737085    -0.753265      89.41
 H      -4.726755    -1.414720    -1.356940      22.55
 O      -3.138821    -2.716998    -1.642351     252.77
 H      -3.605860    -3.554234    -1.534538      20.43
 C      -4.133150    -2.422047     0.525827      87.98
 H      -3.163715    -2.928028     0.883492      19.65
 O      -4.806601    -1.556134     1.371467     409.11
 H      -4.265615    -1.286085     2.008233      32.45
 C      -5.194805    -3.745350     0.372089      74.31
 O      -4.832747    -4.843498    -0.385228     318.92
 H      -4.251022    -5.504683     0.203387      25.13
 H      -6.109638    -3.295888    -0.069137      27.01
 H      -5.137824    -3.939859     1.530798      25.15
55
name = lig-etoh-frame_515
 C       2.010268     1.582337    -1.759964      62.09
 H       1.423856     1.980653    -2.499558      22.02
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 C       3.372795     1.301928     0.255138      38.98
 H       3.907693     1.584583     1.101140      21.46
 C       4.036533     0.126756    -0.225953      16.41
 O       5.034559    -0.623571     0.526853     277.01
 C       6.229596     0.067725     0.598107     112.65
 H       7.039886    -0.127841    -0.175574      26.51
 H       6.687727    -0.278003     1.635873      25.15
 H       6.243424     1.127663     0.529305      30.53
 C       3.519654    -0.494699    -1.538484       1.73
 O       4.198476    -1.482666    -2.158628     148.42
 H       5.302951    -1.307883    -1.893692      21.87
 C       2.615839     0.384048    -2.188355      48.34
 H       2.260356    -0.177375    -3.103187      20.46
 C       2.430021     2.052330    -0.543671      35.45
 C       2.079301     3.504973    -0.028659      78.66
 H       2.492586     4.253354    -0.958771      19.55
 O       2.427846     3.910868     1.325337     302.85
 H       3.367262     4.081528     1.261326      26.63
 C       0.420426     3.560966    -0.135493      67.25
 H       0.141713     3.318098    -1.161599      20.52
 C      -0.322389     4.806475     0.255044      99.60
 O       0.114221     6.140356    -0.209078     282.16
 H       0.568728     5.948720    -1.011176      32.22
 H      -0.308619     4.826958     1.442137      22.82
 H      -1.424643     4.478170     0.131439      22.85
 C      -1.479986    -0.937198    -0.299024      28.74
 H      -1.281018    -1.957082    -0.503604      19.01
 C      -3.382727     0.597896    -0.104090      62.17
 H      -4.276260     1.281432    -0.509317      17.18
 C      -2.534267     1.625964     0.365931      11.40
 O      -3.075465     2.830273     0.612220     134.48
 C      -4.501376     2.788702     1.479891      84.34
 H      -3.996098     2.113794     2.407570      24.28
 H      -4.592669     3.770791     1.758495      26.71
 H      -5.469525     2.355169     1.203655      27.37
 C      -1.117705     1.407365     0.277253      11.60
 O      -0.129622     2.355943     0.695288     136.44
 C      -0.607274     0.083393     0.122670      41.20
 H       0.255925    -0.222693     0.482862      20.10
 C      -2.934129    -0.586925    -0.610689      20.45
 C      -3.872435    -1.663452    -0.795449      86.20
 H      -4.889506    -1.518839    -1.283086      24.49
 O      -3.149974    -2.764066    -1.598814     173.17
 H      -3.910901    -3.524281    -1.382365      17.19
 C      -4.065531    -2.444343     0.478537      93.17
 H      -3.167952    -2.889451     0.845201      24.00
 O      -4.804593    -1.568635     1.269087     327.91
 H      -4.180086    -1.197289     2.100892      23.10
 C      -5.152874    -3.604948     0.359279     109.99
 O      -4.803819    -4.827788    -0.366208     338.75
 H      -4.288737    -5.364663     0.189646      31.02
 H      -6.254141    -3.375725     0.204036      26.23
 H      -5.321540    -4.193287     1.290827      24.55
55
name = lig-etoh-frame_516
 C       2.033625     1.635215    -1.718975      31.93
 H       1.327370     2.131416    -2.490770      17.83
 C       3.420488     1.322450     0.229725      57.59
 H       3.970042     1.805687     1.131942      15.02
 C       3.955180     0.050723    -0.150581      -1.37
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 O       5.027487    -0.555104     0.549482     295.38
 C       6.257676    -0.008178     0.631858     117.44
 H       6.947911    -0.232274    -0.177437      28.39
 H       6.829013    -0.249106     1.566727      26.29
 H       6.343595     1.147704     0.637189      29.23
 C       3.556290    -0.459485    -1.532606       6.95
 O       4.204635    -1.545873    -2.169331     209.84
 H       5.044094    -1.479119    -2.003064      24.72
 C       2.579545     0.344636    -2.147654      44.31
 H       2.282936     0.056235    -3.213385      24.53
 C       2.441470     2.091930    -0.487868      37.96
 C       1.962509     3.487749    -0.022636     109.69
 H       2.371517     4.181558    -0.736846      23.74
 O       2.436365     3.901724     1.242712     280.22
 H       3.393240     4.246230     1.230103      27.20
 C       0.449391     3.591522    -0.137964      74.71
 H       0.177131     3.405873    -1.216103      21.02
 C      -0.355271     4.775043     0.341750     109.91
 O       0.161829     6.099067    -0.221308     226.74
 H       0.435134     5.953565    -1.248472      27.94
 H      -0.163465     5.016458     1.352966      24.93
 H      -1.461155     4.667816     0.509355      23.50
 C      -1.581869    -0.960147    -0.292181      42.13
 H      -1.256606    -1.986087    -0.638868      16.92
 C      -3.378678     0.596607    -0.068884      80.44
 H      -4.152115     1.065795    -0.549104      21.30
 C      -2.560762     1.599238     0.427366       2.22
 O      -3.107721     2.839561     0.644348     173.79
 C      -4.519162     2.848063     1.465734      98.56
 H      -4.304433     2.555209     2.438173      28.06
 H      -4.622135     3.967374     1.788882      24.31
 H      -5.401138     2.235028     1.009594      25.98
 C      -1.121261     1.437434     0.226307      -2.28
 O      -0.100352     2.382162     0.693573     126.63
 C      -0.615824     0.058900     0.101572      14.65
 H       0.580007    -0.112376     0.387191      16.36
 C      -2.807483    -0.522408    -0.633057      25.94
 C      -3.931626    -1.690144    -0.899537      65.39
 H      -4.981095    -1.407864    -1.224859      23.13
 O      -3.193476    -2.813626    -1.568689     234.35
 H      -3.734222    -3.571134    -1.525117      20.93
 C      -4.074413    -2.490271     0.432603      90.84
 H      -3.046303    -2.773583     0.921981      20.53
 O      -4.801660    -1.546931     1.237333     334.27
 H      -4.252949    -1.176669     2.021330      24.38
 C      -5.124049    -3.528407     0.393325     105.94
 O      -4.782861    -4.804377    -0.395728     326.40
 H      -4.080400    -5.258537     0.246472      25.89
 H      -6.178405    -3.238999     0.209668      27.06
 H      -5.370232    -3.970695     1.405037      25.71
55
name = lig-etoh-frame_517
 C       2.069973     1.613953    -1.715731      21.06
 H       1.347472     2.258378    -2.223955      18.00
 C       3.489966     1.343325     0.228882      49.29
 H       3.795132     1.917902     1.060838      15.84
 C       3.874823    -0.005059    -0.138601      15.15
 O       4.955990    -0.517068     0.569270     286.26
 C       6.366905    -0.007214     0.660736      86.32
 H       6.773016    -0.492688    -0.274607      25.70
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 H       6.861441    -0.400308     1.614331      25.54
 H       6.200164     1.040277     0.765899      29.20
 C       3.612425    -0.389629    -1.463757      -5.23
 O       4.153710    -1.587717    -2.180750     102.03
 H       5.326456    -1.840999    -1.935476      16.44
 C       2.529939     0.316836    -2.156046      54.76
 H       2.328355     0.219253    -3.199423      26.20
 C       2.473736     2.136204    -0.409216      18.39
 C       1.868239     3.470110    -0.015074     102.91
 H       2.321788     4.335257    -0.817764      20.11
 O       2.441549     3.896196     1.189663     245.80
 H       3.425832     4.285834     1.056332      25.98
 C       0.414550     3.567226    -0.147074      80.98
 H       0.234639     3.477922    -1.198860      21.43
 C      -0.355967     4.804215     0.469472      94.41
 O       0.207645     6.037430    -0.259128     231.49
 H       0.007163     6.003384    -1.214950      30.47
 H       0.204195     5.073193     1.480684      22.11
 H      -1.518613     4.853267     0.398304      21.80
 C      -1.569428    -0.968231    -0.295560      46.91
 H      -1.173571    -1.964648    -0.617304      16.82
 C      -3.371750     0.634514    -0.074045      56.83
 H      -4.502359     0.731486    -0.510420      17.00
 C      -2.531242     1.595837     0.461968      -1.24
 O      -3.179864     2.871060     0.710387     213.56
 C      -4.488105     2.932885     1.445588     110.13
 H      -4.480182     2.543707     2.606757      25.42
 H      -4.790319     3.987564     1.350956      25.54
 H      -5.129470     2.374862     0.839009      27.29
 C      -1.087842     1.453169     0.237251      -1.41
 O      -0.089242     2.407435     0.684589     155.97
 C      -0.639276     0.050500     0.083064      26.94
 H       0.401156     0.044752     0.041610      18.97
 C      -2.807914    -0.545518    -0.642326      10.42
 C      -3.898402    -1.770494    -0.982108      51.22
 H      -4.878037    -1.225332    -1.318639      22.02
 O      -3.231400    -2.842845    -1.594614     233.83
 H      -3.673136    -3.785508    -1.637242      16.83
 C      -4.106384    -2.460888     0.412431     101.34
 H      -3.177492    -2.675605     0.808167      23.87
 O      -4.809957    -1.498620     1.251557     372.58
 H      -4.259600    -1.207294     1.948860      29.21
 C      -5.125522    -3.562388     0.446869      72.66
 O      -4.761146    -4.765178    -0.415175     334.45
 H      -3.928861    -5.120715     0.060672      27.14
 H      -5.973526    -2.993088    -0.088400      26.94
 H      -5.197184    -3.558888     1.598008      25.90
55
name = lig-etoh-frame_518
 C       2.116775     1.566185    -1.664947      33.89
 H       1.396737     2.187720    -2.204419      18.60
 C       3.501788     1.395431     0.239791      54.89
 H       3.873944     1.789708     1.243771      15.88
 C       3.867868     0.022418    -0.130099      13.56
 O       4.872978    -0.528201     0.616688     241.45
 C       6.428374    -0.008344     0.671847      70.00
 H       6.756260    -0.423179    -0.253730      28.73
 H       6.736758    -0.666233     1.577489      25.36
 H       6.316396     1.096715     0.759571      29.10
 C       3.637681    -0.369048    -1.448377      -5.65
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 O       4.126949    -1.598654    -2.164070     218.36
 H       4.866244    -2.004850    -1.851422      24.32
 C       2.508169     0.334705    -2.163444      48.26
 H       2.380322     0.082786    -3.321310      23.62
 C       2.509155     2.116302    -0.405577      25.73
 C       1.883599     3.499411    -0.047123     106.19
 H       2.057286     4.198537    -0.845006      23.73
 O       2.447926     3.911052     1.182962     305.49
 H       3.316283     4.097446     0.914737      30.57
 C       0.297339     3.527587    -0.118060      73.22
 H       0.070272     3.486126    -1.240965      19.59
 C      -0.280629     4.886263     0.567690     108.64
 O       0.237410     5.975279    -0.300798     248.46
 H      -0.373224     5.976046    -1.095043      29.12
 H       0.147321     4.887561     1.514179      25.93
 H      -1.327123     4.831530     0.403011      23.68
 C      -1.465887    -0.959641    -0.316062      36.39
 H      -1.115991    -1.947756    -0.513344      17.85
 C      -3.393067     0.634353    -0.155562      64.58
 H      -4.445370     0.570191     0.006008      20.31
 C      -2.515928     1.650641     0.465401     -15.09
 O      -3.221414     2.907056     0.798625     237.02
 C      -4.433890     3.008307     1.413636     132.89
 H      -4.640263     2.528145     2.371558      27.64
 H      -4.805362     3.951666     1.036364      25.58
 H      -5.144754     2.364822     0.691042      24.48
 C      -1.058417     1.444622     0.304845      17.89
 O      -0.106228     2.409204     0.668635     196.39
 C      -0.686370     0.105772     0.047461      38.02
 H       0.455446    -0.037664    -0.185806      16.72
 C      -2.915649    -0.632171    -0.627366      -6.18
 C      -3.820904    -1.826505    -0.992466      79.74
 H      -4.672267    -1.361618    -1.570817      22.29
 O      -3.238649    -2.875659    -1.694846     244.58
 H      -3.829059    -3.763176    -1.533980      14.66
 C      -4.162263    -2.357883     0.397367      96.87
 H      -3.085375    -2.702846     0.780844      19.70
 O      -4.829525    -1.439274     1.276332     327.03
 H      -4.071945    -1.186238     2.084479      21.15
 C      -5.131202    -3.597328     0.471745      87.46
 O      -4.738979    -4.711085    -0.407609     355.09
 H      -3.941716    -5.130199    -0.098297      29.71
 H      -5.842880    -3.110829    -0.211101      26.81
 H      -5.293982    -3.649337     1.524281      26.84
55
name = lig-etoh-frame_519
 C       2.133615     1.527229    -1.618539      43.62
 H       1.422679     2.028334    -2.366195      18.63
 C       3.493016     1.435936     0.299348      71.92
 H       3.964712     1.519242     1.274542      15.13
 C       3.928740     0.125058    -0.132755      15.37
 O       4.816845    -0.568589     0.689583     192.19
 C       6.395145    -0.036886     0.676765      93.09
 H       6.921697    -0.250056    -0.305459      30.05
 H       6.709379    -0.654108     1.463564      28.74
 H       6.612386     1.051461     0.798503      30.60
 C       3.604809    -0.399538    -1.497664       3.60
 O       4.053059    -1.562141    -2.134294     144.32
 H       4.833046    -2.064852    -1.521584      19.16
 C       2.566654     0.330277    -2.184160      55.08
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 H       2.344713    -0.041386    -3.102586      24.80
 C       2.532133     2.093582    -0.446548      48.48
 C       1.896629     3.498446    -0.095339      86.31
 H       2.097678     4.281589    -1.030986      21.28
 O       2.434096     3.941234     1.192914     223.71
 H       3.521848     3.962735     0.991709      26.17
 C       0.201163     3.507531    -0.071694      77.75
 H      -0.227571     3.457801    -1.052022      22.32
 C      -0.167907     4.931752     0.581501      97.82
 O       0.259497     5.921193    -0.333132     239.35
 H      -0.615726     5.991558    -0.918708      25.96
 H       0.042096     4.883567     1.744133      24.32
 H      -1.384029     4.796066     0.663676      22.40
 C      -1.458107    -0.923287    -0.374327      28.06
 H      -0.960040    -1.995358    -0.422442      17.65
 C      -3.389803     0.608335    -0.217498      55.91
 H      -4.407919     0.684450     0.373635      19.76
 C      -2.544804     1.694970     0.422029      -8.67
 O      -3.151719     2.930435     0.876950     225.84
 C      -4.467400     3.020047     1.303949     124.76
 H      -4.665970     2.666572     2.404312      26.51
 H      -4.736827     4.160865     1.064827      24.30
 H      -5.181807     2.421957     0.818412      28.36
 C      -1.097517     1.461392     0.397368      17.41
 O      -0.142343     2.380908     0.669994     209.60
 C      -0.661191     0.179469    -0.006032      32.54
 H       0.405099    -0.129717    -0.162983      16.66
 C      -2.937535    -0.728205    -0.579003       6.62
 C      -3.771058    -1.826848    -0.976316      87.08
 H      -4.581544    -1.617734    -1.768060      19.96
 O      -3.222585    -2.927946    -1.822130     250.55
 H      -3.861615    -3.568156    -1.486445      18.40
 C      -4.197371    -2.297326     0.426862     105.30
 H      -3.283438    -2.622383     0.787802      24.51
 O      -4.822211    -1.367967     1.326022     395.63
 H      -4.235465    -1.184835     2.002903      31.98
 C      -5.118579    -3.586939     0.434008      95.98
 O      -4.718181    -4.661861    -0.395345     330.94
 H      -3.917680    -5.272234    -0.016950      25.44
 H      -6.158284    -3.371193    -0.036131      24.79
 H      -5.594997    -4.095244     1.435411      23.69
55
name = lig-etoh-frame_520
 C       2.108640     1.485574    -1.658745      67.83
 H       1.444193     1.972818    -2.289552      22.47
 C       3.499519     1.400958     0.364718       4.72
 H       3.905933     1.638862     1.361987      22.06
 C       4.007988     0.226173    -0.188913      54.90
 O       4.809672    -0.593965     0.754704     219.84
 C       6.315795    -0.080094     0.654365      92.73
 H       6.886866    -0.215856    -0.276101      25.07
 H       6.896148    -0.717019     1.524127      25.22
 H       6.520550     0.944225     0.972996      28.57
 C       3.551602    -0.412343    -1.506903      33.27
 O       3.992335    -1.531475    -2.082850     204.87
 H       4.690660    -1.853525    -1.296886      23.77
 C       2.679276     0.306934    -2.173917      44.72
 H       2.105196    -0.157797    -3.135242      19.47
 C       2.533146     2.132769    -0.467483      44.10
 C       1.891781     3.483102    -0.162304      94.19
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 H       2.259372     4.229307    -0.894318      18.42
 O       2.429635     3.974564     1.182558     329.16
 H       3.376669     3.943502     1.280076      27.50
 C       0.182527     3.524133    -0.013450      67.04
 H      -0.448652     3.473840    -0.967933      20.57
 C      -0.126492     4.887601     0.615686     119.13
 O       0.263244     5.888491    -0.351322     281.09
 H      -0.475721     6.103312    -0.864507      30.61
 H       0.221606     5.170871     1.582959      26.18
 H      -1.166515     4.965625     0.809487      25.95
 C      -1.506553    -0.884271    -0.438780      54.98
 H      -0.988594    -1.757459    -0.482961      20.18
 C      -3.378603     0.600402    -0.204760      67.38
 H      -4.378478     0.738754     0.229653      19.88
 C      -2.588165     1.691555     0.338911       9.88
 O      -3.016156     2.922426     0.934741     192.17
 C      -4.545577     3.046205     1.218179     120.67
 H      -4.524600     3.027540     2.349618      24.83
 H      -4.629678     4.070291     1.231543      26.36
 H      -5.340269     2.360205     0.676408      25.56
 C      -1.188509     1.483270     0.456617       8.24
 O      -0.173458     2.346264     0.723004     203.33
 C      -0.631353     0.216719    -0.062166      16.24
 H       0.455500     0.053069     0.015137      16.53
 C      -2.838270    -0.740659    -0.526183      25.38
 C      -3.783728    -1.829970    -1.000385      74.18
 H      -4.644996    -1.515129    -1.555413      22.90
 O      -3.182584    -2.967395    -1.928831     182.79
 H      -3.855834    -3.786069    -1.563521      13.30
 C      -4.265008    -2.314268     0.491931      83.91
 H      -3.249684    -2.637310     1.011660      19.46
 O      -4.830120    -1.297275     1.356098     332.27
 H      -4.185593    -1.098427     2.186659      24.24
 C      -5.189692    -3.584156     0.406685     112.91
 O      -4.666971    -4.645425    -0.405598     357.93
 H      -4.112004    -5.160940     0.180706      28.48
 H      -6.254258    -3.459890     0.214555      26.60
 H      -5.414635    -4.147491     1.261530      26.98
55
name = lig-etoh-frame_521
 C       2.101463     1.470610    -1.700739      56.88
 H       1.257338     2.053515    -2.279673      18.68
 C       3.483286     1.371529     0.386935      11.11
 H       3.718455     1.895240     1.345344      18.69
 C       4.088884     0.259818    -0.244274      32.99
 O       4.845465    -0.588921     0.776558     252.68
 C       6.237830    -0.158777     0.682957     102.68
 H       6.611463    -0.318456    -0.343717      25.56
 H       6.833661    -0.695841     1.307595      27.45
 H       6.081189     0.893553     1.072853      24.75
 C       3.553391    -0.384348    -1.418084      25.58
 O       3.964828    -1.536603    -1.998241     268.50
 H       4.601132    -1.841843    -1.430297      28.21
 C       2.685771     0.322076    -2.226009      51.60
 H       2.157029    -0.107605    -2.960152      22.75
 C       2.530949     2.147912    -0.484318      16.13
 C       1.892259     3.463709    -0.171629      88.52
 H       2.299446     4.278705    -0.924706      18.42
 O       2.382272     4.001699     1.171141     296.68
 H       3.387939     3.977483     1.241134      27.95
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 C       0.210574     3.535421     0.030616      66.31
 H      -0.329559     3.549639    -0.895194      21.78
 C      -0.114259     4.852856     0.655747      99.85
 O       0.281578     5.874736    -0.357363     205.16
 H      -0.398887     6.161041    -1.019713      28.84
 H       0.670725     5.279600     1.421205      23.35
 H      -1.261871     5.111650     0.908385      23.32
 C      -1.458153    -0.813411    -0.480506      52.42
 H      -0.985185    -1.883968    -0.755277      17.21
 C      -3.363305     0.604832    -0.155866      68.66
 H      -4.519075     0.622676    -0.176087      18.72
 C      -2.618135     1.678363     0.267561      18.23
 O      -2.917549     2.883110     0.966862     159.26
 C      -4.575258     3.076943     1.172442      98.22
 H      -4.577206     2.961914     2.268351      24.74
 H      -4.686477     4.280036     0.999632      24.13
 H      -5.208608     2.514820     0.593865      27.28
 C      -1.236334     1.444073     0.427798      13.21
 O      -0.192694     2.333953     0.828047     169.59
 C      -0.657426     0.253361    -0.090575      34.06
 H       0.479775     0.322713     0.221395      14.24
 C      -2.797099    -0.677200    -0.515243      20.72
 C      -3.801275    -1.855491    -1.001889      34.44
 H      -4.764690    -1.220409    -1.306021      20.56
 O      -3.170433    -2.985165    -1.984895     216.39
 H      -3.486694    -3.816556    -1.832054      21.34
 C      -4.308728    -2.383479     0.572479      73.32
 H      -3.450679    -2.709072     1.074269      19.89
 O      -4.844944    -1.230861     1.379956     307.76
 H      -4.173804    -1.093226     2.209481      22.23
 C      -5.289998    -3.591521     0.418196      68.77
 O      -4.612373    -4.637228    -0.439116     344.04
 H      -4.141753    -5.121893     0.283935      25.36
 H      -6.320244    -3.265454     0.096948      26.59
 H      -5.045954    -3.981625     1.568250      24.06
55
name = lig-etoh-frame_522
 C       2.087075     1.530710    -1.729796      45.95
 H       1.292641     1.935318    -2.233791      19.05
 C       3.421759     1.407495     0.331263      24.35
 H       3.660602     1.876340     1.260606      20.02
 C       4.153629     0.239442    -0.213769      44.52
 O       4.858468    -0.589875     0.753351     262.60
 C       6.140516    -0.205013     0.710545      77.97
 H       6.364361    -0.252282    -0.400521      22.60
 H       6.905413    -0.914250     1.365521      23.11
 H       6.074026     0.840135     0.977668      24.76
 C       3.592246    -0.329462    -1.328061      12.82
 O       3.940217    -1.562926    -1.904332     173.92
 H       4.917267    -2.115128    -1.501367      21.63
 C       2.638415     0.376737    -2.251021      32.61
 H       2.192076    -0.246855    -3.174633      20.48
 C       2.538048     2.089804    -0.505058      21.38
 C       1.889609     3.472686    -0.120773      93.35
 H       2.080495     4.233871    -0.990531      19.32
 O       2.329003     4.014793     1.158374     284.78
 H       3.368560     4.100343     0.941162      25.33
 C       0.267992     3.507736     0.069122      58.14
 H      -0.144318     3.501461    -0.988652      18.89
 C      -0.107910     4.906336     0.699662     109.55
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 O       0.305960     5.883366    -0.362347     209.18
 H      -0.321090     5.930913    -1.234834      26.59
 H       0.763270     4.967050     1.337694      24.45
 H      -1.054140     4.957437     1.064343      27.12
 C      -1.335927    -0.803367    -0.531622      51.46
 H      -1.086817    -1.689564    -0.937802      19.18
 C      -3.411900     0.581453    -0.119338      92.36
 H      -4.403183     0.598187    -0.687963      17.84
 C      -2.608681     1.697693     0.260549      11.70
 O      -2.902104     2.834584     0.973820     157.52
 C      -4.510603     3.178782     1.147267      97.94
 H      -4.859884     2.677481     2.194273      23.68
 H      -4.713439     4.065203     0.722383      27.54
 H      -5.102489     2.498228     0.381611      25.81
 C      -1.217017     1.404937     0.338056      16.37
 O      -0.221760     2.343122     0.951543     144.14
 C      -0.658638     0.305138    -0.068579      55.22
 H       0.329699     0.287365     0.124557      17.04
 C      -2.825523    -0.615272    -0.555001      -9.69
 C      -3.810902    -1.864583    -0.932450      43.30
 H      -4.631712    -1.360998    -1.338069      23.65
 O      -3.168274    -2.919386    -2.012892     177.40
 H      -3.366409    -3.950368    -1.835627      17.62
 C      -4.349251    -2.429408     0.603269      65.71
 H      -3.430833    -2.893339     1.156137      18.45
 O      -4.856772    -1.197147     1.390498     326.56
 H      -4.252558    -1.069190     2.079767      26.84
 C      -5.335698    -3.600271     0.492090      86.86
 O      -4.582697    -4.617948    -0.456297     313.08
 H      -4.021209    -5.253568     0.209672      24.69
 H      -6.256458    -3.253862     0.005310      27.48
 H      -5.313346    -3.803789     1.472416      29.73
55
name = lig-etoh-frame_523
 C       2.080014     1.589045    -1.770111      45.91
 H       1.189856     2.046154    -2.351544      16.14
 C       3.398462     1.437604     0.245160      43.22
 H       3.707553     1.768144     1.272189      25.10
 C       4.144549     0.227675    -0.104750      97.73
 O       4.786742    -0.618915     0.719890     294.76
 C       6.139807    -0.224722     0.716457     115.54
 H       6.508435    -0.181385    -0.310797      26.77
 H       6.660016    -0.874250     1.263735      26.86
 H       6.490080     0.852074     1.011880      25.43
 C       3.632821    -0.295793    -1.336805      39.22
 O       3.943891    -1.617745    -1.793573     193.81
 H       4.818222    -1.857578    -1.701194      28.95
 C       2.605979     0.389094    -2.228409      23.82
 H       2.444407    -0.126292    -3.150091      23.16
 C       2.509120     2.061826    -0.518354      57.51
 C       1.839081     3.461013    -0.047361     116.73
 H       1.935580     4.177721    -0.952296      22.85
 O       2.326415     4.019521     1.124884     288.87
 H       3.208814     4.273029     0.973494      31.03
 C       0.317589     3.457707     0.093080      66.10
 H      -0.040541     3.273062    -0.919384      18.87
 C      -0.044267     4.938800     0.683864      95.72
 O       0.310839     5.905807    -0.367615     280.01
 H      -0.070504     5.550732    -1.149207      30.72
 H       0.620484     4.937837     1.592307      24.30
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 H      -1.114625     4.850666     1.305871      22.96
 C      -1.339009    -0.790145    -0.586940      43.46
 H      -0.893621    -1.766738    -1.049820      17.34
 C      -3.478202     0.563722    -0.150395     100.52
 H      -4.374190     0.813561    -0.701602      16.21
 C      -2.578934     1.697472     0.295709       3.18
 O      -2.962289     2.815564     0.978489     199.11
 C      -4.415749     3.174609     1.093542     116.33
 H      -4.930445     2.862872     1.932847      28.45
 H      -4.632243     4.290686     0.638625      25.09
 H      -4.782447     2.541712     0.341275      30.98
 C      -1.190408     1.496167     0.286001      16.10
 O      -0.268310     2.367049     1.051831     155.69
 C      -0.595959     0.265888    -0.067685      23.50
 H       0.608070     0.119122    -0.048092      15.64
 C      -2.796907    -0.620866    -0.614451      -0.70
 C      -3.780172    -1.869724    -0.824226      60.89
 H      -4.692320    -1.648952    -1.587932      19.89
 O      -3.179113    -2.809105    -2.006702     212.07
 H      -3.437031    -3.718466    -1.576253      17.79
 C      -4.343180    -2.431824     0.605717      80.56
 H      -3.506714    -2.875301     1.120029      22.91
 O      -4.879468    -1.216671     1.362837     280.86
 H      -4.114488    -0.966109     2.187398      19.37
 C      -5.329925    -3.595393     0.521137      79.75
 O      -4.577151    -4.598999    -0.428476     324.23
 H      -4.022554    -5.206131    -0.013556      29.88
 H      -6.260297    -3.418451    -0.046291      26.05
 H      -5.917465    -4.062822     1.616187      23.48
55
name = lig-etoh-frame_524
 C       2.055687     1.628409    -1.833503      26.30
 H       1.342701     2.199401    -2.401527      18.87
 C       3.465588     1.424676     0.232247      30.74
 H       3.644902     1.806613     1.223681      13.95
 C       4.006820     0.232245    -0.071975      14.82
 O       4.715558    -0.642228     0.711101     250.82
 C       6.203222    -0.202638     0.700288     104.22
 H       6.752353    -0.305796    -0.308207      28.01
 H       6.647435    -1.130301     1.380775      25.78
 H       6.549166     0.675665     1.218710      29.43
 C       3.656529    -0.278995    -1.397065      13.40
 O       3.927399    -1.651406    -1.691441     161.70
 H       5.063535    -1.658131    -1.718832      19.60
 C       2.646487     0.374489    -2.150429      54.06
 H       2.521979    -0.024349    -3.210032      24.97
 C       2.417260     2.119466    -0.540659      73.67
 C       1.786977     3.405311    -0.002272     110.64
 H       1.934474     4.154657    -0.917065      22.06
 O       2.350043     4.023641     1.114585     229.81
 H       3.341188     4.395970     1.091086      29.02
 C       0.331055     3.411956     0.150212      58.20
 H      -0.143214     3.101012    -0.809345      18.57
 C       0.005363     4.905071     0.681833     102.24
 O       0.299967     5.924140    -0.342869     270.77
 H       0.163857     5.319044    -1.180195      28.50
 H       0.457644     5.247001     1.666285      24.92
 H      -0.992723     4.962870     0.936153      25.84
 C      -1.404281    -0.787071    -0.643517      49.13
 H      -0.825547    -1.691462    -0.775295      20.01
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 C      -3.460519     0.582317    -0.220729      27.82
 H      -4.576312     0.989211    -0.392016      17.11
 C      -2.576090     1.649511     0.335159      -6.60
 O      -3.035546     2.826155     1.001384     217.82
 C      -4.308568     3.166323     0.959248     116.38
 H      -4.937370     3.145710     2.043229      23.32
 H      -4.314153     4.202795     0.889191      25.32
 H      -4.814707     2.552777     0.146316      25.19
 C      -1.118034     1.593481     0.290508       1.17
 O      -0.322229     2.409395     1.108178     184.67
 C      -0.493641     0.204326    -0.097063       2.66
 H       0.502342     0.087060    -0.148215      18.10
 C      -2.786453    -0.662630    -0.657541      22.67
 C      -3.758989    -1.850914    -0.793885      88.37
 H      -4.632995    -1.703149    -1.300294      22.10
 O      -3.195812    -2.694612    -1.937786     268.68
 H      -3.497380    -3.484590    -1.526911      19.84
 C      -4.322320    -2.398488     0.620591      85.11
 H      -3.412329    -2.788217     1.195580      20.92
 O      -4.877263    -1.268763     1.337961     386.18
 H      -4.321084    -1.005481     2.000602      29.67
 C      -5.349763    -3.631998     0.541011     102.45
 O      -4.604686    -4.564491    -0.387063     352.40
 H      -3.929002    -5.228714     0.108516      24.87
 H      -6.185246    -3.452743    -0.190796      26.81
 H      -5.872666    -4.112873     1.196586      27.41
55
name = lig-etoh-frame_525
 C       2.063656     1.654272    -1.841637      30.09
 H       1.455783     2.240653    -2.579446      17.38
 C       3.479362     1.476224     0.255973      60.16
 H       3.635187     1.933829     1.238823      13.13
 C       3.846169     0.188884    -0.129610       4.32
 O       4.697332    -0.632858     0.715534     221.42
 C       6.285240    -0.266991     0.718281     103.93
 H       6.708192    -0.370396    -0.236041      30.91
 H       6.564384    -1.077712     1.258929      29.47
 H       6.292904     0.660113     1.355348      28.25
 C       3.640846    -0.284163    -1.429024      30.77
 O       3.946769    -1.664285    -1.601987     198.06
 H       5.022922    -1.621763    -1.742571      20.67
 C       2.703948     0.365349    -2.124801      51.98
 H       2.467742     0.046275    -3.189588      24.12
 C       2.365302     2.158207    -0.556815      50.61
 C       1.794851     3.353952    -0.003391     110.33
 H       1.911837     4.125510    -0.892666      20.82
 O       2.392073     4.033538     1.149182     244.36
 H       3.391066     4.148455     0.978180      29.69
 C       0.293507     3.398151     0.245776      70.37
 H      -0.249166     3.240551    -0.708231      18.14
 C       0.015914     4.874781     0.676529     101.27
 O       0.290723     5.916491    -0.317993     239.34
 H       0.387110     5.560596    -1.278357      28.88
 H       0.448968     5.317920     1.526802      25.79
 H      -1.195012     5.004690     0.502300      21.02
 C      -1.414278    -0.763817    -0.654380      42.58
 H      -0.971431    -1.790660    -0.641061      20.09
 C      -3.381950     0.644994    -0.286733      55.92
 H      -4.407986     0.692526    -0.058597      21.58
 C      -2.563383     1.594722     0.369293     -10.09
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 O      -3.020299     2.793189     1.021178     214.54
 C      -4.315673     3.181925     0.854431     124.16
 H      -4.701281     3.102709     1.793340      27.18
 H      -4.144504     4.370700     0.810203      24.19
 H      -5.064195     2.884891     0.088700      27.24
 C      -1.042986     1.555290     0.323649      -2.05
 O      -0.365373     2.470815     1.138130     210.80
 C      -0.503434     0.223739    -0.142555      11.04
 H       0.676156     0.033575    -0.166195      14.94
 C      -2.854170    -0.665972    -0.662787       7.05
 C      -3.743064    -1.814113    -0.810218      60.96
 H      -4.888886    -1.288759    -1.026882      21.23
 O      -3.208287    -2.594688    -1.828813     206.93
 H      -3.576139    -3.644239    -1.713449      15.68
 C      -4.277825    -2.388024     0.678110      80.29
 H      -3.394687    -2.703978     1.268476      21.10
 O      -4.897764    -1.334312     1.289219     356.97
 H      -4.286778    -0.991874     2.126514      23.00
 C      -5.332875    -3.640136     0.440117      70.42
 O      -4.622557    -4.556644    -0.337017     353.97
 H      -4.018091    -5.028159     0.313698      24.61
 H      -6.081821    -3.214142    -0.237762      27.07
 H      -5.783923    -4.304632     1.492566      23.75
55
name = lig-etoh-frame_526
 C       2.111799     1.648241    -1.815588      48.93
 H       1.562314     2.092801    -2.685939      18.19
 C       3.398844     1.549178     0.257241      68.23
 H       3.746670     1.946251     1.239456      13.31
 C       3.777309     0.155674    -0.136447      13.62
 O       4.698904    -0.600917     0.710755     228.91
 C       6.281809    -0.341127     0.758614      68.05
 H       6.667626    -0.224223    -0.337207      29.75
 H       6.689471    -1.265115     1.384949      25.77
 H       6.156150     0.666889     1.226213      27.63
 C       3.600571    -0.345591    -1.406040      32.49
 O       3.987283    -1.663740    -1.548663     224.91
 H       4.919662    -1.809043    -1.666256      23.88
 C       2.698731     0.419538    -2.210321      41.53
 H       2.423395    -0.027104    -3.139860      23.38
 C       2.408991     2.131305    -0.545216      46.04
 C       1.804260     3.370127    -0.006669      96.58
 H       1.802062     4.163235    -0.858432      20.40
 O       2.442513     4.018916     1.183913     263.50
 H       3.407564     3.945859     0.951646      27.56
 C       0.247799     3.434797     0.319622      88.42
 H      -0.227721     3.477608    -0.680643      19.70
 C      -0.080762     4.870690     0.616873     107.73
 O       0.318494     5.919321    -0.313357     293.77
 H       0.387893     5.788941    -1.218661      32.45
 H       0.393906     5.191775     1.647440      24.71
 H      -1.105356     4.819236     0.626046      26.06
 C      -1.413314    -0.750806    -0.631685      39.69
 H      -1.188383    -1.863255    -0.688630      20.47
 C      -3.292583     0.690042    -0.323697      55.60
 H      -4.340901     0.397866     0.190290      16.90
 C      -2.482831     1.578868     0.391945       5.59
 O      -2.941464     2.699268     1.008379     154.77
 C      -4.379383     3.295796     0.771273      91.30
 H      -4.870837     2.908958     1.842699      23.44
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 H      -4.216635     4.322694     0.567028      26.66
 H      -5.079122     3.051312    -0.041480      27.55
 C      -1.034855     1.415278     0.374334       9.97
 O      -0.394959     2.520608     1.159797     210.47
 C      -0.537902     0.298041    -0.186361      51.66
 H       0.479145     0.002250    -0.097802      17.36
 C      -2.867909    -0.588519    -0.632780      -6.69
 C      -3.824110    -1.741619    -0.806463      76.77
 H      -4.644227    -1.177745    -0.938911      26.19
 O      -3.226030    -2.557983    -1.733009     287.16
 H      -3.601232    -3.380945    -1.902869      22.74
 C      -4.219768    -2.428155     0.715727      81.54
 H      -3.344972    -2.765726     1.328979      20.99
 O      -4.927067    -1.367915     1.275088     361.13
 H      -4.436048    -1.047744     2.151914      23.62
 C      -5.299940    -3.614028     0.377726      98.25
 O      -4.623304    -4.588415    -0.302173     414.39
 H      -4.035778    -4.967994     0.333975      30.93
 H      -6.138948    -3.023952    -0.100372      29.85
 H      -5.525628    -3.882477     1.282171      29.69
55
name = lig-etoh-frame_527
 C       2.178281     1.601119    -1.822704      64.19
 H       1.522916     2.093723    -2.502767      20.34
 C       3.328363     1.517376     0.257410      29.10
 H       3.760562     1.895692     1.143549      16.69
 C       3.811297     0.192040    -0.071295      13.70
 O       4.698698    -0.572150     0.708550     267.50
 C       6.200254    -0.398401     0.774123     115.80
 H       6.616710    -0.206606    -0.158494      30.80
 H       6.750571    -1.132330     1.346448      27.63
 H       6.396024     0.588970     1.203949      28.81
 C       3.528162    -0.403475    -1.360916      19.09
 O       4.003055    -1.674179    -1.535566      78.78
 H       5.146270    -1.992342    -1.536342      20.02
 C       2.698270     0.451202    -2.316200      45.51
 H       2.333453    -0.127553    -3.283419      19.67
 C       2.464335     2.135279    -0.509757      33.00
 C       1.781276     3.445198     0.012790      89.05
 H       1.817104     4.227655    -0.847521      17.99
 O       2.481150     3.976876     1.196425     253.61
 H       3.571815     3.958182     1.106775      24.92
 C       0.236332     3.486826     0.300053      84.17
 H      -0.167082     3.378373    -0.749379      19.70
 C      -0.181046     4.901399     0.599896     106.84
 O       0.361587     5.939914    -0.284923     217.22
 H       0.160081     5.713505    -1.328568      24.81
 H       0.150688     5.070344     1.567236      25.84
 H      -1.392026     4.790725     0.909648      22.33
 C      -1.454920    -0.759212    -0.603412      60.18
 H      -1.104527    -1.729367    -0.803982      20.57
 C      -3.279258     0.709485    -0.287458      60.93
 H      -4.219256     0.675799     0.109526      20.25
 C      -2.388474     1.581477     0.378342      21.79
 O      -2.891567     2.633154     0.985997     103.89
 C      -4.437797     3.366908     0.736529      74.29
 H      -5.016964     3.103333     1.500455      26.71
 H      -4.234473     4.473137     0.573503      24.74
 H      -4.823299     2.867092    -0.229326      24.85
 C      -1.082170     1.354419     0.474586       4.67
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 O      -0.417745     2.526295     1.173608     199.04
 C      -0.558688     0.295690    -0.234664      48.31
 H       0.507790     0.037877    -0.055445      17.16
 C      -2.776282    -0.511553    -0.603196      18.56
 C      -3.870595    -1.659771    -0.719484      47.01
 H      -4.952704    -1.195737    -1.233910      20.90
 O      -3.228651    -2.540547    -1.686467     229.74
 H      -3.843060    -3.316421    -1.901065      19.86
 C      -4.177554    -2.465021     0.671991      93.94
 H      -3.310250    -2.857698     1.296282      20.25
 O      -4.968502    -1.379623     1.306345     355.95
 H      -4.588050    -1.110739     2.101171      28.66
 C      -5.222606    -3.490693     0.350860      79.34
 O      -4.628180    -4.656914    -0.307384     327.27
 H      -3.873145    -5.130918     0.315995      24.34
 H      -6.150022    -3.136299    -0.089482      28.32
 H      -5.650655    -3.679049     1.586017      25.07
55
name = lig-etoh-frame_528
 C       2.220232     1.590148    -1.830017      34.81
 H       1.362654     2.243205    -2.273188      17.97
 C       3.336694     1.396339     0.314635      36.55
 H       3.698260     1.932435     1.251115      21.83
 C       3.886072     0.231036    -0.051525      30.34
 O       4.705407    -0.555795     0.735107     269.63
 C       6.086685    -0.385664     0.777302     105.47
 H       6.613825    -0.402428    -0.289847      24.19
 H       6.616980    -1.232053     1.339254      25.08
 H       6.611270     0.476019     1.344457      25.07
 C       3.457094    -0.407714    -1.302880      21.97
 O       4.029267    -1.718048    -1.555202     217.85
 H       4.891805    -1.667440    -1.416663      27.62
 C       2.739856     0.365946    -2.387968      35.86
 H       2.369548     0.050433    -3.286655      20.02
 C       2.446146     2.193422    -0.527690      30.03
 C       1.785071     3.523711     0.041763     101.18
 H       1.983520     4.292296    -0.832022      19.64
 O       2.513580     3.927636     1.207460     309.19
 H       3.418887     4.105905     1.124836      31.93
 C       0.230082     3.510318     0.198304      60.63
 H      -0.119833     3.113251    -0.764561      21.03
 C      -0.318597     4.941146     0.628269     106.58
 O       0.382489     5.947905    -0.267582     241.11
 H      -0.140494     5.654600    -1.035822      29.10
 H       0.137469     5.207574     1.691842      24.66
 H      -1.346094     5.022452     0.749097      26.19
 C      -1.428366    -0.768647    -0.583175      61.02
 H      -0.881613    -1.709023    -0.983786      17.31
 C      -3.274905     0.742881    -0.208515      40.66
 H      -4.421295     1.106444    -0.102196      16.78
 C      -2.412206     1.594213     0.330066      21.13
 O      -2.899386     2.661417     1.000884     120.43
 C      -4.426045     3.379853     0.644113      70.92
 H      -5.286037     3.225734     1.516851      23.24
 H      -4.168245     4.497387     0.712386      24.05
 H      -4.517718     2.855271    -0.241638      24.84
 C      -1.049841     1.378549     0.580412      -5.69
 O      -0.420137     2.498526     1.179084     186.60
 C      -0.544827     0.235201    -0.242539      26.22
 H       0.602147     0.125910    -0.164282      16.61
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 C      -2.774895    -0.495580    -0.581005      38.60
 C      -3.877982    -1.579057    -0.658047      93.02
 H      -4.736979    -1.459391    -1.128185      24.15
 O      -3.235073    -2.543035    -1.664805     205.81
 H      -4.071958    -3.218159    -1.762657      19.17
 C      -4.165546    -2.407013     0.577093     109.17
 H      -3.324815    -2.822264     1.104030      22.59
 O      -5.015253    -1.397186     1.345460     293.41
 H      -4.515534    -1.116324     2.333864      21.80
 C      -5.155992    -3.425596     0.424789     107.29
 O      -4.642199    -4.731112    -0.310090     331.59
 H      -3.934891    -5.158519     0.145740      30.43
 H      -6.012921    -3.263168    -0.300902      27.57
 H      -5.625886    -3.639315     1.247901      28.49
55
name = lig-etoh-frame_529
 C       2.216649     1.635052    -1.819100      22.73
 H       1.467134     2.130509    -2.355121      19.56
 C       3.333076     1.371857     0.400326      23.77
 H       3.566045     1.783225     1.345198      23.05
 C       3.950071     0.213760    -0.100132      35.92
 O       4.694143    -0.546691     0.789710     278.20
 C       6.069070    -0.373563     0.765153     113.54
 H       6.414679    -0.554250    -0.205378      27.31
 H       6.210685    -1.403178     1.233751      23.82
 H       6.408780     0.446698     1.320011      26.56
 C       3.419631    -0.409581    -1.298747      22.50
 O       4.009078    -1.736765    -1.587025     149.52
 H       5.029556    -1.419261    -1.284850      16.91
 C       2.792645     0.282404    -2.334121      37.94
 H       2.446396     0.054180    -3.460126      19.03
 C       2.442463     2.189941    -0.549316      31.48
 C       1.837368     3.571433     0.040187     102.86
 H       2.042815     4.363333    -0.744055      20.92
 O       2.496468     3.882832     1.239805     242.35
 H       3.491289     4.285819     0.922585      25.40
 C       0.208517     3.518571     0.114819      33.05
 H      -0.150106     3.051638    -0.844893      20.16
 C      -0.369033     4.983829     0.677980      95.39
 O       0.355753     5.937350    -0.241074     194.63
 H      -0.199547     5.864204    -1.045138      28.52
 H       0.015435     5.198207     1.613182      26.28
 H      -1.567182     5.232663     0.458325      22.88
 C      -1.351419    -0.794815    -0.589200      39.91
 H      -1.007415    -1.681075    -0.975404      18.01
 C      -3.337098     0.749473    -0.149462      45.92
 H      -4.251262     1.108607    -0.475594      17.65
 C      -2.449871     1.670870     0.340804       0.57
 O      -2.958581     2.768931     1.044336     181.03
 C      -4.356197     3.360102     0.603583     105.46
 H      -5.148612     3.144775     1.227888      27.89
 H      -4.097971     4.354846     0.636548      27.83
 H      -4.512467     3.037609    -0.515307      26.03
 C      -0.985565     1.395826     0.605277      -3.66
 O      -0.383103     2.464447     1.177265     175.87
 C      -0.487705     0.238333    -0.156801      32.21
 H       0.526966     0.100780    -0.368090      16.94
 C      -2.869909    -0.511445    -0.548354      19.06
 C      -3.788324    -1.557124    -0.658744      80.02
 H      -4.947927    -1.241215    -1.095773      21.62
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 O      -3.267224    -2.558755    -1.648543     254.93
 H      -3.882710    -3.213903    -1.702886      23.05
 C      -4.166079    -2.266094     0.528377      91.53
 H      -3.163667    -2.656747     0.996430      20.77
 O      -5.037273    -1.409221     1.420706     321.13
 H      -4.498879    -1.232846     2.154517      27.44
 C      -5.124227    -3.476547     0.406827      75.26
 O      -4.679630    -4.774761    -0.310186     292.95
 H      -3.872835    -5.220582     0.175733      24.72
 H      -5.752766    -3.165530    -0.429958      26.18
 H      -5.754763    -3.820760     1.469560      23.35
55
name = lig-etoh-frame_530
 C       2.222869     1.642114    -1.816599      42.60
 H       1.594888     2.058077    -2.713854      18.87
 C       3.301284     1.399821     0.416024      30.50
 H       3.489828     1.628263     1.507151      21.82
 C       3.946097     0.206763    -0.131691      54.94
 O       4.626581    -0.535657     0.842124     251.39
 C       6.077028    -0.434443     0.766113      81.88
 H       6.457761    -0.459990    -0.330474      25.14
 H       6.300141    -1.367784     1.277137      24.85
 H       6.314811     0.602877     1.274286      24.47
 C       3.451291    -0.456109    -1.336372      17.67
 O       3.988181    -1.709319    -1.611356     167.21
 H       5.035299    -1.719686    -1.335072      22.29
 C       2.779120     0.297372    -2.239640      49.39
 H       2.725337    -0.100795    -3.189073      19.36
 C       2.474950     2.143807    -0.520082      46.50
 C       1.871963     3.557349    -0.001166     101.43
 H       2.059315     4.512283    -0.718015      19.78
 O       2.478707     3.862329     1.275442     285.12
 H       3.335949     4.200032     1.023344      28.85
 C       0.185317     3.527312     0.098108      44.34
 H      -0.222357     3.320656    -0.886998      20.69
 C      -0.399239     5.005168     0.635187     101.79
 O       0.307576     5.931105    -0.205306     206.24
 H      -0.059708     6.177784    -1.159297      26.45
 H      -0.164798     5.139366     1.778351      24.23
 H      -1.431591     5.148294     0.380884      25.37
 C      -1.364657    -0.763780    -0.572962      25.40
 H      -1.122251    -1.841032    -0.947295      18.30
 C      -3.385359     0.735358    -0.133905      49.65
 H      -4.391621     0.974489    -0.679869      15.62
 C      -2.445763     1.758673     0.428295      -8.88
 O      -3.040331     2.897785     1.074367     219.52
 C      -4.219119     3.311081     0.521908     109.93
 H      -5.142117     2.864104     1.158663      24.57
 H      -4.100557     4.537617     0.562853      23.70
 H      -4.568427     3.321910    -0.489988      27.17
 C      -1.001462     1.405044     0.551637       5.71
 O      -0.294778     2.449824     1.164829     173.55
 C      -0.440154     0.258986    -0.035126      36.76
 H       0.641260     0.092869    -0.492912      16.06
 C      -2.847931    -0.498381    -0.501196       0.69
 C      -3.797497    -1.583618    -0.784331      84.02
 H      -4.611487    -0.960009    -0.990875      23.98
 O      -3.285834    -2.561243    -1.639090     255.26
 H      -3.808989    -3.490817    -1.624017      15.73
 C      -4.171522    -2.177263     0.602255      78.99
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 H      -3.217576    -2.345288     1.033751      22.11
 O      -5.037155    -1.427195     1.474343     330.80
 H      -4.359593    -1.186657     2.273310      22.19
 C      -5.118204    -3.588765     0.354707      95.78
 O      -4.710672    -4.795855    -0.298212     342.84
 H      -3.923878    -5.224359     0.241718      25.33
 H      -5.827001    -3.043399    -0.337599      27.60
 H      -5.525729    -3.722619     1.227004      27.71
55
name = lig-etoh-frame_531
 C       2.245197     1.592439    -1.852102      46.78
 H       1.842830     2.125647    -2.668869      20.69
 C       3.279930     1.398976     0.364459       7.11
 H       3.406447     1.560943     1.424575      20.25
 C       3.871589     0.215676    -0.109944      40.60
 O       4.552278    -0.533449     0.881016     255.54
 C       6.075160    -0.485318     0.760876     103.79
 H       6.476674    -0.324269    -0.226046      27.20
 H       6.752546    -1.207592     1.412946      25.33
 H       6.382916     0.448607     1.120793      27.42
 C       3.565002    -0.481608    -1.316044       9.25
 O       3.974781    -1.699352    -1.649231     221.42
 H       4.851662    -1.963014    -1.464832      25.49
 C       2.727277     0.373601    -2.135907      57.93
 H       2.786817    -0.218967    -3.163287      20.04
 C       2.492578     2.134194    -0.477975      78.00
 C       1.867600     3.516104    -0.048045     105.77
 H       2.084415     4.353620    -0.721100      21.85
 O       2.425254     3.846286     1.307722     241.46
 H       3.472190     4.109596     1.225696      27.15
 C       0.185615     3.551924     0.147270      59.77
 H      -0.298259     3.542388    -0.883222      18.79
 C      -0.385964     4.969360     0.552973     103.94
 O       0.282638     5.969980    -0.164135     264.47
 H      -0.042807     6.132594    -1.042044      30.64
 H      -0.382383     5.134751     1.614287      25.91
 H      -1.611183     4.937281     0.409723      22.55
 C      -1.420355    -0.697471    -0.515548      59.93
 H      -1.128765    -1.686065    -0.804466      19.94
 C      -3.380888     0.769282    -0.133766      47.03
 H      -4.428281     0.846761    -0.455854      20.23
 C      -2.474544     1.775459     0.520646     -12.62
 O      -3.047102     2.988118     1.080468     224.29
 C      -4.172203     3.349488     0.458852     125.96
 H      -4.952998     2.769040     0.933281      26.37
 H      -4.352955     4.324484     0.702897      27.28
 H      -4.337640     3.240815    -0.682369      26.31
 C      -1.071401     1.463403     0.494188      -0.96
 O      -0.178230     2.455684     1.119728     165.52
 C      -0.427345     0.224901     0.028154      31.64
 H       0.577288     0.256973    -0.167685      19.02
 C      -2.722936    -0.481365    -0.464557      11.90
 C      -3.839669    -1.592549    -0.874380      48.97
 H      -4.686010    -0.848346    -1.331560      20.78
 O      -3.303435    -2.588831    -1.666299     241.07
 H      -3.630325    -3.529711    -1.354840      15.19
 C      -4.193317    -2.169404     0.682474      57.42
 H      -3.172518    -2.208824     1.277708      17.69
 O      -5.012305    -1.439960     1.526813     297.97
 H      -4.450407    -1.014312     2.343048      21.65
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 C      -5.097338    -3.626475     0.270418      81.72
 O      -4.726029    -4.813964    -0.292308     351.39
 H      -4.063669    -5.236191     0.241068      29.25
 H      -6.037779    -3.191212    -0.140548      26.78
 H      -5.539061    -3.768808     1.473153      24.24
55
name = lig-etoh-frame_532
 C       2.276586     1.593871    -1.828955      33.31
 H       1.825066     2.318808    -2.552367      15.96
 C       3.264098     1.380463     0.307233      21.83
 H       3.390598     1.660270     1.341111      14.27
 C       3.809999     0.166583    -0.053993      23.73
 O       4.522641    -0.551288     0.925247     262.63
 C       6.077949    -0.503622     0.770498     108.44
 H       6.379227    -0.501968    -0.320212      30.54
 H       6.723628    -1.108287     1.314843      28.66
 H       6.419386     0.545219     1.188739      29.26
 C       3.665750    -0.402548    -1.252152      43.40
 O       3.942174    -1.713225    -1.715754     152.84
 H       4.996666    -2.167643    -1.466997      16.82
 C       2.732371     0.331944    -2.096746      71.32
 H       2.512126     0.030073    -3.115268      26.63
 C       2.457961     2.164230    -0.501083      85.36
 C       1.838804     3.457776    -0.037784      98.47
 H       2.206334     4.241114    -0.927249      21.23
 O       2.363968     3.844501     1.318826     252.22
 H       3.399893     3.861593     1.343371      28.63
 C       0.226039     3.577561     0.188475      81.38
 H      -0.216567     3.353072    -0.777410      19.38
 C      -0.408631     4.899536     0.484657     111.45
 O       0.269401     6.038421    -0.117774     267.49
 H      -0.120750     5.939559    -1.030501      30.01
 H      -0.346229     5.215210     1.584412      25.50
 H      -1.473780     4.715062     0.326295      24.99
 C      -1.368601    -0.648651    -0.427651      63.28
 H      -1.006346    -1.640351    -0.742324      18.90
 C      -3.298517     0.812795    -0.105278      78.40
 H      -4.415167     0.880029    -0.082531      23.02
 C      -2.548710     1.750365     0.580983      -1.45
 O      -2.952207     3.030685     1.077625     202.84
 C      -4.225920     3.404478     0.360258      83.44
 H      -5.088496     2.654684     0.703869      23.17
 H      -4.680084     4.408401     0.879373      23.83
 H      -3.880189     3.154970    -0.658044      25.07
 C      -1.102169     1.539677     0.470224      -8.52
 O      -0.079792     2.467419     1.039785     166.60
 C      -0.511391     0.241054     0.079029      25.85
 H       0.659177     0.291484     0.240160      14.09
 C      -2.735593    -0.440580    -0.465681      21.60
 C      -3.861071    -1.519253    -0.881089      62.56
 H      -4.659323    -1.269290    -1.569349      20.55
 O      -3.313526    -2.641138    -1.707629     283.68
 H      -3.503737    -3.409670    -1.235399      19.83
 C      -4.196911    -2.209480     0.703886      69.23
 H      -3.290025    -2.405780     1.182360      20.20
 O      -5.008729    -1.431622     1.577471     361.99
 H      -4.503658    -1.047995     2.265892      29.12
 C      -5.129514    -3.585921     0.335362     105.73
 O      -4.730703    -4.837794    -0.322386     331.92
 H      -4.037137    -5.383458     0.326670      24.17
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 H      -6.098820    -3.406173    -0.157981      26.68
 H      -5.359002    -3.908758     1.239879      26.68
55
name = lig-etoh-frame_533
 C       2.293137     1.658711    -1.768548      23.70
 H       1.638023     2.250650    -2.471405      17.73
 C       3.236948     1.384447     0.294949      27.44
 H       3.458755     1.810070     1.319694      14.09
 C       3.809439     0.094695     0.063054      -3.71
 O       4.541644    -0.587867     0.987458     283.89
 C       6.061196    -0.446038     0.760206      83.86
 H       6.164462    -0.767731    -0.292604      28.00
 H       6.463317    -1.422499     1.364019      24.15
 H       6.305924     0.522572     1.096923      29.30
 C       3.697642    -0.347068    -1.282267      33.30
 O       3.937613    -1.733990    -1.775707     239.54
 H       4.769318    -1.917082    -1.501247      25.23
 C       2.765710     0.273647    -2.105841      46.33
 H       2.337020     0.050727    -3.127557      24.00
 C       2.413336     2.166399    -0.548771      54.04
 C       1.822912     3.450714    -0.005593     105.57
 H       2.144326     4.130775    -0.795511      22.16
 O       2.299223     3.842832     1.303656     313.26
 H       3.220249     3.767040     1.255557      30.55
 C       0.318512     3.553111     0.153998      82.07
 H      -0.026013     3.098116    -0.819757      18.42
 C      -0.405547     4.859707     0.501758      96.98
 O       0.228661     6.100035    -0.100471     230.53
 H       0.042559     5.874828    -1.123508      27.42
 H      -0.285293     5.101100     1.568695      24.09
 H      -1.528480     4.727369     0.104243      20.77
 C      -1.314392    -0.683138    -0.361423      25.94
 H      -0.856003    -1.669456    -0.698837      16.50
 C      -3.252825     0.830411    -0.060165      94.70
 H      -4.343595     0.911241     0.293161      23.02
 C      -2.533652     1.773571     0.626366       5.51
 O      -2.873041     3.048565     1.065224     167.03
 C      -4.295938     3.439853     0.312185      97.09
 H      -5.029756     2.618021     0.275389      24.73
 H      -4.627667     4.342500     0.628968      27.35
 H      -3.788400     3.481622    -0.665063      25.43
 C      -1.089438     1.605880     0.489034      11.40
 O      -0.030742     2.459355     0.970795     186.90
 C      -0.574064     0.382257     0.169375      31.39
 H       0.390528     0.072858     0.522195      15.53
 C      -2.836644    -0.397023    -0.513330      17.42
 C      -3.821058    -1.472262    -0.832912      69.73
 H      -4.765610    -1.409795    -1.492594      19.83
 O      -3.309421    -2.675457    -1.746556     206.77
 H      -3.407198    -3.554146    -1.091537      14.80
 C      -4.249948    -2.267175     0.641505      61.69
 H      -3.215926    -2.751452     1.012358      15.89
 O      -5.027122    -1.429227     1.595771     286.14
 H      -4.239150    -1.091249     2.387970      17.48
 C      -5.168202    -3.541021     0.431836      83.43
 O      -4.707672    -4.857836    -0.357566     292.80
 H      -4.094041    -5.335276     0.173076      28.87
 H      -6.055841    -3.356263    -0.223490      26.34
 H      -5.391549    -4.055547     1.543847      24.10
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name = lig-etoh-frame_534
 C       2.274341     1.663234    -1.794278      27.93
 H       1.530868     2.017713    -2.479123      19.66
 C       3.233337     1.379181     0.349922      30.82
 H       3.493026     1.832886     1.258534      15.34
 C       3.811877     0.073926     0.148834     -23.54
 O       4.581282    -0.625948     1.062778     284.08
 C       5.997871    -0.462936     0.758706     110.92
 H       6.150236    -0.716964    -0.267941      31.62
 H       6.214403    -1.265830     1.337310      25.71
 H       6.384147     0.608219     0.984027      29.22
 C       3.671286    -0.378821    -1.359689       8.16
 O       3.924874    -1.713986    -1.819158     133.59
 H       4.956400    -1.882587    -1.497142      19.16
 C       2.776284     0.333129    -2.137132      36.76
 H       2.383886    -0.253918    -3.071870      21.47
 C       2.403447     2.147377    -0.511402      41.64
 C       1.822952     3.479866     0.034599     100.95
 H       2.104687     4.422978    -0.727706      19.00
 O       2.240741     3.845809     1.276326     234.65
 H       3.339620     3.837389     1.200980      24.80
 C       0.391734     3.481104     0.033291      81.67
 H       0.116372     3.249521    -1.000405      19.42
 C      -0.380898     4.851849     0.519468      93.36
 O       0.170792     6.129911    -0.110151     263.42
 H       0.297735     6.028803    -1.021644      33.05
 H      -0.386000     4.888644     1.617366      23.67
 H      -1.407954     4.889714     0.036119      21.31
 C      -1.358742    -0.704587    -0.318084      18.14
 H      -0.830008    -1.587127    -0.552464      16.19
 C      -3.295092     0.839249     0.028495      91.84
 H      -4.292712     0.853570     0.316467      21.96
 C      -2.404227     1.854642     0.640039      13.58
 O      -2.869223     3.061123     1.044763     158.95
 C      -4.282896     3.447506     0.243402      75.90
 H      -4.987925     2.628722     0.080929      24.52
 H      -4.633142     4.534006     0.615091      23.31
 H      -3.978907     3.927478    -0.757781      23.95
 C      -1.065176     1.696643     0.551539      33.15
 O      -0.022226     2.437062     0.952125     211.76
 C      -0.621575     0.440418     0.252885      18.19
 H       0.338491     0.061071     0.651137      16.00
 C      -2.841444    -0.397289    -0.569060       9.57
 C      -3.808529    -1.527562    -0.777432      77.71
 H      -4.748542    -1.088086    -1.112423      22.64
 O      -3.292946    -2.694687    -1.750044     256.59
 H      -3.330245    -3.527960    -1.279815      18.62
 C      -4.296745    -2.339952     0.556605      94.94
 H      -3.403930    -2.748911     0.884491      22.21
 O      -4.991964    -1.433111     1.611394     373.21
 H      -4.363582    -1.273850     2.217491      28.35
 C      -5.215122    -3.559336     0.528318      89.48
 O      -4.691578    -4.828474    -0.392680     279.92
 H      -3.947998    -5.340050     0.162919      24.97
 H      -6.052832    -3.199127    -0.040607      28.09
 H      -5.505835    -3.815658     1.488371      28.51
55
name = lig-etoh-frame_535
 C       2.228231     1.611850    -1.853610      36.51
 H       1.389144     1.951014    -2.586069      17.84
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 C       3.257286     1.344475     0.434433      20.02
 H       3.523734     1.832959     1.435660      14.74
 C       3.789515     0.085672     0.121405      -2.91
 O       4.595286    -0.638855     1.122375     268.26
 C       5.926030    -0.482667     0.757459     115.41
 H       6.243885    -0.595744    -0.346983      30.48
 H       6.561609    -1.219245     1.520979      24.42
 H       6.442743     0.483306     0.929040      31.20
 C       3.617353    -0.435268    -1.358447      14.13
 O       3.940665    -1.671793    -1.839984     123.38
 H       4.969534    -2.013354    -1.688874      18.86
 C       2.781399     0.413367    -2.182657      41.75
 H       2.533172    -0.263649    -2.974011      22.92
 C       2.431467     2.126936    -0.451372      72.41
 C       1.869587     3.541418     0.001865     116.42
 H       2.095859     4.418086    -0.630630      23.41
 O       2.242291     3.858136     1.283039     289.12
 H       3.167290     4.093806     1.293892      29.73
 C       0.377127     3.444769    -0.093919      76.86
 H       0.066201     3.397974    -1.155102      20.27
 C      -0.324818     4.855809     0.466794      92.45
 O       0.122229     6.151625    -0.083296     262.27
 H       0.431878     6.021351    -1.049888      30.53
 H      -0.461121     4.792319     1.607005      23.59
 H      -1.406402     4.821324     0.142697      22.70
 C      -1.453508    -0.628152    -0.269359      46.95
 H      -0.868633    -1.633314    -0.413041      14.55
 C      -3.299744     0.825658     0.124819      74.16
 H      -4.498551     0.863943     0.240815      14.87
 C      -2.355023     1.928334     0.590595      11.44
 O      -2.943879     3.104209     1.007842     195.33
 C      -4.204837     3.530175     0.168032      98.03
 H      -4.972077     2.658340     0.068158      22.35
 H      -4.677066     4.171143     0.927575      25.23
 H      -4.055905     3.983349    -0.784049      26.65
 C      -1.014708     1.729269     0.614389      16.43
 O      -0.002081     2.460132     0.965140     200.41
 C      -0.663204     0.337802     0.300315      22.67
 H       0.452339     0.293159     0.623365      15.48
 C      -2.768285    -0.413094    -0.554466      19.83
 C      -3.841065    -1.644368    -0.731733      70.47
 H      -4.688088    -0.882152    -0.972028      19.72
 O      -3.278981    -2.658068    -1.744708     254.15
 H      -3.431593    -3.568246    -1.358572      16.49
 C      -4.317523    -2.386362     0.512496      92.67
 H      -3.295142    -2.678102     1.063007      19.04
 O      -4.953451    -1.464536     1.568210     294.26
 H      -4.176975    -1.291484     2.398835      18.79
 C      -5.261004    -3.594867     0.529443      71.25
 O      -4.683413    -4.758837    -0.391168     287.51
 H      -3.916145    -5.218408     0.126933      24.77
 H      -6.272679    -3.226677     0.116362      26.29
 H      -5.607420    -3.783010     1.684758      24.86
55
name = lig-etoh-frame_536
 C       2.150758     1.590466    -1.847668      65.92
 H       1.488213     2.048186    -2.500161      22.82
 C       3.273684     1.332599     0.511547      22.39
 H       3.509477     1.661300     1.481640      23.78
 C       3.774694     0.065601     0.028598      23.52
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 O       4.565462    -0.629928     1.141149     237.76
 C       5.956980    -0.526219     0.774024     118.59
 H       6.131602    -0.701195    -0.243927      27.50
 H       6.706479    -0.990225     1.273758      25.92
 H       6.282683     0.557833     1.031468      25.96
 C       3.555879    -0.430655    -1.261118      41.08
 O       3.971946    -1.644863    -1.865533     255.43
 H       4.826936    -1.915166    -1.739950      27.38
 C       2.825099     0.414153    -2.209673      44.38
 H       2.562526    -0.091801    -3.301646      17.23
 C       2.482844     2.102736    -0.449312      41.29
 C       1.922192     3.553769    -0.075090      97.99
 H       2.329365     4.433253    -0.847941      20.27
 O       2.256277     3.888137     1.329388     272.94
 H       3.149516     4.326949     1.336447      25.97
 C       0.337450     3.499046    -0.162163      76.55
 H      -0.099698     3.204168    -1.156945      19.92
 C      -0.295303     4.842493     0.375106      97.80
 O       0.094152     6.166384    -0.042849     280.85
 H       0.383304     5.940452    -1.001901      30.28
 H      -0.194802     4.895396     1.431961      24.69
 H      -1.452951     4.593203     0.264298      21.58
 C      -1.469502    -0.597795    -0.221722      60.06
 H      -1.157692    -1.564806    -0.359926      17.25
 C      -3.271385     0.789815     0.182094      49.87
 H      -4.256006     0.962451     0.156068      14.74
 C      -2.433821     1.965115     0.503066      -3.65
 O      -3.049991     3.169542     0.944034     234.08
 C      -4.132924     3.592380     0.162003     116.75
 H      -4.766182     2.780268     0.024993      28.06
 H      -4.686669     4.010898     1.071526      23.43
 H      -3.895738     4.058224    -0.872708      25.27
 C      -0.991300     1.620272     0.642879       1.16
 O       0.048955     2.541401     0.975560     175.17
 C      -0.642372     0.286142     0.366348      47.69
 H       0.389108     0.196382     0.404704      18.10
 C      -2.788901    -0.413224    -0.445494      13.05
 C      -3.865269    -1.712442    -0.720871      79.54
 H      -4.691931    -1.213463    -1.206974      21.27
 O      -3.274409    -2.587918    -1.722789     253.17
 H      -3.754286    -3.551632    -1.494213      14.71
 C      -4.278286    -2.419376     0.577623      99.52
 H      -3.416079    -2.715638     1.077916      22.25
 O      -4.892721    -1.501709     1.512588     419.52
 H      -4.291946    -1.262123     2.235137      29.10
 C      -5.320951    -3.634237     0.497862      90.79
 O      -4.693871    -4.659265    -0.358205     370.49
 H      -3.998963    -5.078039     0.136865      28.90
 H      -6.305019    -3.475376     0.132679      26.99
 H      -5.363047    -3.954995     1.542965      27.46
55
name = lig-etoh-frame_537
 C       2.128612     1.564318    -1.754223      59.16
 H       1.565716     2.316676    -2.481214      21.74
 C       3.259533     1.318867     0.491819      32.73
 H       3.531036     1.553747     1.543923      24.02
 C       3.784876     0.048340     0.019218      31.19
 O       4.512455    -0.627485     1.116051     242.69
 C       6.012349    -0.502952     0.785900      69.68
 H       6.026057    -0.823262    -0.314025      24.43
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 H       6.800389    -1.235143     1.362451      21.45
 H       6.037737     0.589731     0.946591      25.67
 C       3.498171    -0.413741    -1.219339      15.58
 O       3.977217    -1.612891    -1.887077     163.83
 H       5.093694    -1.797872    -1.547669      19.94
 C       2.843537     0.383053    -2.244528      21.48
 H       2.732410     0.203385    -3.242607      17.59
 C       2.528754     2.091237    -0.469999      37.80
 C       1.977988     3.535066    -0.161154      89.11
 H       2.486037     4.205632    -0.847868      19.62
 O       2.271234     3.924202     1.353242     249.62
 H       3.189885     4.501741     1.261539      22.97
 C       0.334355     3.584049    -0.180218      74.56
 H      -0.123179     3.015959    -0.964699      22.14
 C      -0.315823     4.810706     0.317880     101.18
 O       0.081716     6.164191    -0.035957     296.40
 H       0.224080     6.145482    -0.957917      33.36
 H       0.187495     4.879104     1.377015      21.40
 H      -1.358731     4.633960     0.258455      24.89
 C      -1.464085    -0.653580    -0.186303      29.68
 H      -1.198321    -1.763349    -0.453899      16.67
 C      -3.229555     0.797583     0.195521      39.26
 H      -4.395899     1.075608     0.131180      17.47
 C      -2.499540     1.936407     0.430739       5.40
 O      -3.091473     3.202107     0.881605     230.04
 C      -4.112181     3.653527     0.175399     117.85
 H      -4.720747     2.712612    -0.286255      24.85
 H      -4.816585     4.346644     0.799856      24.42
 H      -3.760737     4.255534    -0.635961      27.22
 C      -1.022394     1.547012     0.664555      -1.71
 O       0.072569     2.617796     0.965874      90.96
 C      -0.563773     0.298357     0.437877      42.62
 H       0.529764    -0.144595     0.222702      14.83
 C      -2.904358    -0.425627    -0.287204      16.09
 C      -3.860557    -1.708240    -0.735694      65.88
 H      -4.847270    -1.538513    -1.351949      18.84
 O      -3.277725    -2.544368    -1.693413     282.75
 H      -3.826792    -3.257530    -1.713268      23.93
 C      -4.267451    -2.445403     0.671794      59.62
 H      -3.290907    -3.038157     1.090656      17.04
 O      -4.857695    -1.526168     1.443090     356.94
 H      -4.223068    -1.183180     2.222031      23.89
 C      -5.316345    -3.667773     0.460948      78.29
 O      -4.718276    -4.563718    -0.337829     355.51
 H      -3.944143    -5.078359     0.219376      22.75
 H      -6.388114    -3.550199     0.045642      25.63
 H      -5.270544    -4.203970     1.522474      24.78
55
name = lig-etoh-frame_538
 C       2.168346     1.544561    -1.672696      75.68
 H       1.796284     2.260156    -2.304748      25.24
 C       3.245179     1.288314     0.413775      29.44
 H       3.514018     1.601873     1.431042      25.05
 C       3.796784     0.063417     0.116540      36.48
 O       4.465735    -0.643956     1.060382     243.43
 C       6.038465    -0.486597     0.779933      97.69
 H       6.145164    -0.766101    -0.238594      28.65
 H       6.413614    -1.200107     1.430805      24.44
 H       6.244227     0.590381     0.829663      28.22
 C       3.459417    -0.432676    -1.305851      20.79
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 O       4.021371    -1.578457    -1.874563     210.92
 H       4.834512    -1.700425    -1.492416      24.38
 C       2.804052     0.405075    -2.196799      40.04
 H       2.982098     0.248861    -3.431681      16.75
 C       2.539025     2.094536    -0.467180      53.21
 C       1.999863     3.486565    -0.179060      92.12
 H       2.714087     4.227784    -0.894267      16.96
 O       2.300677     3.972199     1.313897     304.93
 H       3.117782     4.365412     1.235057      28.41
 C       0.391778     3.605390    -0.183133      69.49
 H      -0.063922     3.034516    -1.059030      22.40
 C      -0.302021     4.820338     0.329195      93.56
 O       0.078818     6.165951    -0.059866     248.72
 H      -0.015645     6.431124    -1.061361      28.99
 H       0.092282     4.699756     1.281591      25.08
 H      -1.527789     4.797998     0.350562      20.76
 C      -1.502796    -0.755347    -0.137936      24.69
 H      -1.056367    -1.645197    -0.511182      18.13
 C      -3.326577     0.859838     0.175934      26.61
 H      -4.342622     1.016163     0.203629      19.72
 C      -2.468110     1.897868     0.418797      10.73
 O      -3.042579     3.172622     0.859635     213.97
 C      -4.189300     3.731072     0.115004     122.68
 H      -4.680929     3.074407    -0.484542      29.01
 H      -4.822182     4.497831     0.551556      25.57
 H      -3.673387     4.523939    -0.582260      24.23
 C      -1.050761     1.611942     0.680803     -12.50
 O       0.045596     2.655833     0.955737     120.98
 C      -0.484202     0.228387     0.436805       6.73
 H       0.491711    -0.061214     0.378563      17.02
 C      -2.957165    -0.514875    -0.151618      20.56
 C      -3.885515    -1.663051    -0.718732      61.12
 H      -4.899745    -1.428249    -1.002643      21.15
 O      -3.230404    -2.510118    -1.683319     222.76
 H      -3.955724    -3.263762    -1.935201      19.46
 C      -4.251617    -2.520979     0.708836      91.34
 H      -3.424058    -3.077905     1.003736      21.67
 O      -4.839748    -1.511748     1.422475     378.37
 H      -4.214210    -1.086406     2.216191      23.62
 C      -5.299798    -3.665348     0.498785      99.41
 O      -4.701646    -4.541883    -0.375438     406.58
 H      -4.008480    -5.024385     0.042856      30.56
 H      -6.249823    -3.357106     0.130377      28.32
 H      -5.560695    -4.200043     1.462966      26.71
55
name = lig-etoh-frame_539
 C       2.236615     1.552870    -1.641972      53.66
 H       1.776371     2.264059    -2.442508      21.05
 C       3.255000     1.279103     0.383977      24.78
 H       3.475590     1.781053     1.306900      20.62
 C       3.755357     0.056884     0.122021      24.16
 O       4.469875    -0.669422     0.999839     237.28
 C       5.990118    -0.465373     0.766789     100.77
 H       6.364445    -0.784916    -0.257310      26.54
 H       6.275063    -1.170272     1.647301      23.53
 H       6.602498     0.534509     0.920814      27.71
 C       3.468891    -0.448209    -1.359599       6.87
 O       4.051468    -1.546647    -1.862246     132.45
 H       4.953598    -1.797315    -1.331130      18.20
 C       2.761555     0.421587    -2.173877      55.08
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 H       2.955725     0.241310    -3.100178      22.96
 C       2.509306     2.097035    -0.436183      49.43
 C       2.026945     3.484633    -0.134487     111.88
 H       2.503872     4.176806    -0.768291      21.16
 O       2.315108     4.003311     1.224128     276.20
 H       3.385155     4.234390     1.196458      24.62
 C       0.457280     3.549651    -0.212388      70.03
 H       0.126373     3.318347    -1.204642      22.42
 C      -0.307658     4.880634     0.348893      96.30
 O       0.095245     6.187572    -0.098692     264.59
 H      -0.377257     6.374102    -0.983390      29.18
 H      -0.150792     4.792924     1.523261      23.49
 H      -1.302222     4.770904     0.368894      24.46
 C      -1.529804    -0.810955    -0.047969      32.40
 H      -0.989762    -1.676711    -0.533969      15.67
 C      -3.445140     0.847463     0.129783      37.69
 H      -4.586095     1.060089     0.273141      21.39
 C      -2.405171     1.893003     0.463368      -0.34
 O      -2.984665     3.126215     0.844042     133.30
 C      -4.206445     3.852809    -0.000884      75.35
 H      -4.858551     3.213497    -0.778762      23.47
 H      -4.892424     4.470337     0.830047      22.38
 H      -3.652046     4.510891    -0.617638      24.93
 C      -1.005776     1.673575     0.664467     -14.49
 O      -0.027550     2.652039     0.946580     178.85
 C      -0.544127     0.182533     0.392862       4.61
 H       0.654964     0.121035     0.602056      14.15
 C      -2.939730    -0.591280    -0.060705      28.60
 C      -3.907511    -1.646581    -0.622173      41.92
 H      -4.912432    -1.057425    -0.772421      21.38
 O      -3.181007    -2.476799    -1.694367     210.46
 H      -3.871322    -3.160897    -2.004033      21.01
 C      -4.260981    -2.587929     0.680772      87.99
 H      -3.232773    -3.005521     1.159053      17.57
 O      -4.835345    -1.466790     1.456909     396.93
 H      -4.280908    -1.167827     2.164917      27.82
 C      -5.287818    -3.631008     0.570144      80.45
 O      -4.685028    -4.566630    -0.469076     337.82
 H      -3.907613    -5.093596    -0.054293      25.92
 H      -6.181915    -3.048961     0.097819      28.21
 H      -5.769185    -4.093954     1.554982      26.40
55
name = lig-etoh-frame_540
 C       2.265094     1.639531    -1.705953      55.41
 H       1.708547     2.140302    -2.459438      16.91
 C       3.272698     1.320909     0.429383      58.53
 H       3.569394     1.855484     1.383628      11.74
 C       3.674943     0.011373     0.000875       1.84
 O       4.526868    -0.689319     0.937446     277.52
 C       5.953322    -0.472564     0.790189     138.36
 H       6.416447    -0.883455    -0.105539      30.53
 H       6.362376    -1.073130     1.606536      27.55
 H       6.404429     0.446958     1.072116      31.05
 C       3.513604    -0.427452    -1.300660      24.51
 O       4.100696    -1.536382    -1.860141     128.33
 H       4.908114    -1.986252    -1.227970      16.66
 C       2.745091     0.387011    -2.131748      54.56
 H       2.731846     0.158643    -3.390160      25.45
 C       2.467812     2.096734    -0.399342      66.91
 C       2.016237     3.502908    -0.040041      92.69
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 H       2.254291     4.341531    -0.989404      22.82
 O       2.363145     4.034973     1.127881     273.48
 H       3.368208     3.959929     1.177167      28.45
 C       0.500466     3.525309    -0.198096      53.40
 H       0.216835     3.423091    -1.288542      17.80
 C      -0.261665     4.931546     0.407241      77.27
 O       0.106658     6.215619    -0.144855     276.30
 H      -0.507994     6.195392    -0.830947      31.60
 H      -0.265393     5.087886     1.449777      24.31
 H      -1.452079     4.598101     0.112325      17.96
 C      -1.501704    -0.829556     0.056905      45.71
 H      -1.179899    -1.807278    -0.381406      14.65
 C      -3.475204     0.772673     0.100903      60.76
 H      -4.514466     1.090614     0.267141      25.00
 C      -2.421607     1.872164     0.510487     -16.62
 O      -2.952428     3.104261     0.810202      92.45
 C      -4.202969     3.939182    -0.092805      82.85
 H      -4.831473     3.348249    -0.657366      28.67
 H      -4.632168     4.186892     0.799102      25.26
 H      -3.579503     4.545166    -0.673294      25.65
 C      -0.951672     1.639973     0.602946       1.96
 O      -0.113317     2.626485     0.920161     200.00
 C      -0.647087     0.224502     0.359809      31.35
 H       0.363285     0.131117     0.626820      15.93
 C      -2.922798    -0.580480    -0.013922      26.10
 C      -3.909103    -1.671995    -0.487309      65.27
 H      -4.668174    -0.996193    -0.867062      22.10
 O      -3.157994    -2.415600    -1.703084     244.02
 H      -3.740345    -3.083592    -1.927000      24.15
 C      -4.223326    -2.580556     0.681605     108.86
 H      -3.330219    -2.761911     1.192996      21.22
 O      -4.858504    -1.438783     1.492952     325.02
 H      -4.146619    -1.261133     2.394603      20.02
 C      -5.292138    -3.604880     0.586360      85.53
 O      -4.694969    -4.601636    -0.550920     285.02
 H      -3.875457    -5.091901    -0.094569      23.95
 H      -6.004430    -3.056270     0.032067      29.66
 H      -5.742622    -4.005105     1.555692      27.70
55
name = lig-etoh-frame_541
 C       2.279618     1.694315    -1.794988      29.02
 H       1.589516     2.238624    -2.499273      16.42
 C       3.280708     1.360882     0.482158      68.54
 H       3.712981     1.602679     1.425907      15.84
 C       3.644483     0.005622    -0.040007      10.50
 O       4.572491    -0.708144     0.861718     266.42
 C       5.943562    -0.505053     0.844361      99.41
 H       6.385991    -0.864730    -0.078738      28.04
 H       6.469990    -1.157825     1.627444      26.29
 H       5.986525     0.687086     1.087059      25.45
 C       3.560121    -0.422459    -1.270039      22.33
 O       4.156872    -1.547576    -1.851625     253.60
 H       4.712134    -1.942828    -1.323227      24.59
 C       2.730316     0.364579    -2.160677      39.22
 H       2.429437     0.083433    -3.055072      25.42
 C       2.449713     2.113350    -0.378999      59.06
 C       1.952235     3.529345    -0.054756     102.18
 H       2.131490     4.170904    -0.921690      24.67
 O       2.436801     4.071539     1.097054     308.91
 H       3.391577     3.969124     1.127353      29.93
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 C       0.497700     3.568835    -0.112379      64.21
 H       0.172440     3.256654    -1.092314      18.87
 C      -0.244179     4.937926     0.423469      93.76
 O       0.115090     6.236112    -0.189678     232.68
 H      -0.532326     6.213036    -1.016342      28.32
 H      -0.204057     5.148039     1.548491      22.74
 H      -1.102625     4.709012     0.028137      22.80
 C      -1.515526    -0.835135     0.148743      48.66
 H      -1.263340    -1.862764    -0.039342      16.94
 C      -3.376746     0.720973     0.119347      57.07
 H      -4.444932     0.976550     0.163827      26.00
 C      -2.495982     1.809122     0.516726      -6.24
 O      -2.936489     3.103527     0.759284     130.64
 C      -4.152285     3.951429    -0.143375      54.45
 H      -4.868211     3.219384    -0.671481      24.58
 H      -4.553078     4.240224     1.005548      20.62
 H      -3.430147     4.705610    -0.694013      22.13
 C      -1.022851     1.555182     0.507334      24.35
 O      -0.169707     2.604824     0.882464     205.97
 C      -0.717567     0.302649     0.350874      45.26
 H       0.373563    -0.038545     0.484142      16.89
 C      -2.912961    -0.534043    -0.000660      26.34
 C      -3.839382    -1.691619    -0.412072      69.29
 H      -4.705807    -1.273943    -1.015822      21.25
 O      -3.150845    -2.326827    -1.688067     189.23
 H      -3.740082    -3.256640    -1.803875      18.22
 C      -4.202692    -2.495765     0.735846     101.76
 H      -3.219949    -2.831115     1.278245      18.87
 O      -4.872966    -1.433245     1.561292     386.97
 H      -4.374697    -1.247799     2.274733      31.22
 C      -5.262637    -3.603747     0.521613      79.14
 O      -4.723723    -4.631259    -0.589396     302.14
 H      -3.998797    -5.035988    -0.186692      29.31
 H      -6.146563    -3.176639    -0.083298      27.63
 H      -5.590880    -4.065988     1.509499      26.21
55
name = lig-etoh-frame_542
 C       2.293704     1.686322    -1.834533      17.06
 H       1.609871     2.324584    -2.441295      15.06
 C       3.268809     1.342514     0.478244      54.09
 H       3.744234     1.433656     1.506671      16.00
 C       3.708097     0.066642     0.064946      12.94
 O       4.551371    -0.758964     0.792204     284.81
 C       5.957498    -0.483981     0.899486     105.22
 H       6.444334    -0.595679    -0.132589      27.85
 H       6.414592    -1.120436     1.702800      26.60
 H       5.977811     0.524073     0.980613      32.37
 C       3.568944    -0.436919    -1.359838      -0.36
 O       4.178305    -1.541369    -1.861354     147.13
 H       4.879245    -2.061701    -1.099207      17.63
 C       2.706944     0.399789    -2.163466      47.62
 H       2.181337    -0.204994    -3.142541      20.16
 C       2.464317     2.144680    -0.400364      71.00
 C       1.899032     3.519539    -0.105485      97.68
 H       2.274006     4.178450    -1.094052      22.20
 O       2.504809     4.116402     1.121834     228.89
 H       3.623740     4.195304     0.962385      25.36
 C       0.412080     3.621662     0.019260      82.70
 H       0.037956     3.220500    -0.947966      16.64
 C      -0.190858     4.947947     0.414293      92.44
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 O       0.116576     6.246407    -0.238043     264.60
 H      -0.186961     6.313295    -1.189437      30.45
 H      -0.121628     4.967782     1.519608      23.92
 H      -1.384093     4.777709     0.067469      17.58
 C      -1.588606    -0.818030     0.222826      49.86
 H      -1.111367    -1.875716     0.385664      15.77
 C      -3.288758     0.755067     0.172415      49.44
 H      -4.424591     0.775859    -0.059347      19.36
 C      -2.560171     1.764128     0.478855      20.05
 O      -2.934831     3.107837     0.691141     214.98
 C      -4.064807     3.911787    -0.103951     115.80
 H      -4.698505     3.268678    -0.689954      27.45
 H      -4.548034     4.450024     0.589590      27.10
 H      -3.594041     4.573090    -0.704975      27.94
 C      -1.186625     1.583790     0.426283      37.64
 O      -0.208784     2.576603     0.852389     196.57
 C      -0.681996     0.251972     0.350234      32.22
 H       0.429982     0.001223     0.191929      17.79
 C      -2.877914    -0.559379    -0.016538      47.27
 C      -3.747547    -1.655926    -0.453816      68.04
 H      -4.812641    -1.568289    -0.805499      20.18
 O      -3.161927    -2.270502    -1.651177     268.95
 H      -3.502982    -3.166906    -1.611410      19.40
 C      -4.193972    -2.421205     0.852232      83.56
 H      -3.376886    -3.008957     1.284997      21.08
 O      -4.914840    -1.459370     1.601991     340.53
 H      -4.300310    -1.078356     2.521987      20.59
 C      -5.219016    -3.614257     0.393596      91.76
 O      -4.774384    -4.633790    -0.596775     314.47
 H      -3.921042    -5.140345    -0.180584      24.77
 H      -6.215184    -3.342354     0.059094      28.10
 H      -5.367077    -4.244116     1.385641      26.74
55
name = lig-etoh-frame_543
 C       2.297100     1.679191    -1.780313      17.20
 H       1.716791     2.282038    -2.449277      15.54
 C       3.256253     1.298555     0.468144      29.66
 H       3.458509     1.640304     1.479609      16.96
 C       3.807689     0.103806     0.072249      34.61
 O       4.510250    -0.838943     0.754566     255.75
 C       5.974636    -0.446508     0.906979      99.15
 H       6.519253    -0.516937    -0.008558      28.88
 H       6.334981    -1.020589     1.739476      27.54
 H       6.223306     0.744528     1.187310      27.81
 C       3.550766    -0.386859    -1.397131       6.94
 O       4.196946    -1.550825    -1.862186     212.94
 H       4.818654    -1.843672    -1.142376      23.15
 C       2.673753     0.379673    -2.212470      52.21
 H       2.285765    -0.145701    -2.998591      21.89
 C       2.503607     2.154957    -0.471195      76.54
 C       1.916118     3.533138    -0.135910     110.00
 H       2.186291     4.139551    -0.946780      27.37
 O       2.570565     4.154656     1.133662     282.85
 H       3.467242     4.402256     0.905184      30.25
 C       0.291511     3.623186     0.079316      91.53
 H      -0.056325     3.495682    -0.975928      18.39
 C      -0.228893     4.976684     0.370566     118.36
 O       0.144549     6.251556    -0.268919     307.44
 H       0.145093     6.100587    -1.221676      32.67
 H      -0.028761     5.051552     1.471366      25.06
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 H      -1.229550     4.897452     0.475400      26.04
 C      -1.560444    -0.835462     0.313594      50.47
 H      -1.147416    -1.728314     0.563080      15.34
 C      -3.360166     0.709108     0.170801      69.85
 H      -4.322634     0.845141    -0.130170      17.08
 C      -2.579250     1.861370     0.435331      19.70
 O      -2.962958     3.136567     0.619954     280.34
 C      -3.943428     3.815707    -0.043055     103.36
 H      -4.608850     3.188463    -0.692860      25.27
 H      -4.748575     4.697980     0.423925      22.75
 H      -3.514877     4.521671    -0.943478      23.85
 C      -1.244429     1.620854     0.372150      17.54
 O      -0.252744     2.539046     0.852442     218.37
 C      -0.633380     0.202618     0.334780      22.44
 H       0.420574     0.162689     0.137686      16.97
 C      -2.870201    -0.575581    -0.044640      28.97
 C      -3.718896    -1.630245    -0.503268      66.96
 H      -4.782573    -1.295644    -0.608296      22.00
 O      -3.156117    -2.241155    -1.606699     271.26
 H      -3.366426    -3.202354    -1.530223      18.73
 C      -4.201750    -2.413244     0.918430      64.72
 H      -3.437324    -3.018223     1.501661      21.08
 O      -4.947138    -1.488675     1.671732     386.72
 H      -4.389396    -1.108073     2.316586      30.00
 C      -5.167169    -3.654927     0.315576     102.25
 O      -4.798973    -4.626445    -0.600106     349.02
 H      -4.045693    -5.149710    -0.240411      29.35
 H      -6.226318    -3.312456     0.141902      28.07
 H      -5.270419    -4.270595     1.236181      26.92
55
name = lig-etoh-frame_544
 C       2.280354     1.660419    -1.725302      76.51
 H       1.768694     2.277153    -2.545375      19.63
 C       3.228203     1.291845     0.456663      20.96
 H       3.154914     1.872477     1.401783      20.78
 C       3.875894     0.106440    -0.053428      62.07
 O       4.514376    -0.905954     0.747990     245.30
 C       5.985372    -0.363527     0.925417      94.78
 H       6.610238    -0.682961     0.016413      22.74
 H       6.337348    -1.085144     1.786661      24.29
 H       6.055313     0.552039     1.277575      26.85
 C       3.545876    -0.312517    -1.375430      15.42
 O       4.184817    -1.533431    -1.863566     211.79
 H       4.835164    -1.740968    -1.150927      23.59
 C       2.674912     0.345826    -2.223105      43.56
 H       2.295485    -0.089680    -3.307749      17.68
 C       2.561564     2.145470    -0.520108      92.86
 C       1.942850     3.547342    -0.083886      82.82
 H       2.034369     4.407999    -1.024386      21.30
 O       2.542822     4.166330     1.124010     216.55
 H       3.608214     4.501468     0.898159      24.41
 C       0.217480     3.589585     0.020519      65.16
 H      -0.101140     3.562376    -1.012586      17.71
 C      -0.282571     5.048350     0.424466      94.64
 O       0.183522     6.235668    -0.301989     235.53
 H       0.431466     5.783279    -1.229482      28.52
 H       0.214192     5.396926     1.394151      22.81
 H      -1.479657     5.003494     0.666566      22.12
 C      -1.457957    -0.850116     0.395168      34.18
 H      -1.193544    -2.009236     0.569677      12.44
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 C      -3.472919     0.677409     0.132521      75.99
 H      -4.578273     1.003185    -0.189554      14.21
 C      -2.596797     1.934734     0.369054      -0.02
 O      -2.978343     3.192130     0.605139     258.93
 C      -3.905646     3.782967    -0.085728     133.55
 H      -4.566660     3.003916    -0.531803      25.98
 H      -4.474961     4.355849     0.470026      27.78
 H      -3.376690     4.263817    -0.813555      28.39
 C      -1.172134     1.601102     0.342271      10.76
 O      -0.295701     2.515967     0.869222     212.65
 C      -0.647594     0.244361     0.313728      29.54
 H       0.571095     0.277666     0.313260      12.97
 C      -2.860662    -0.539697    -0.041478      22.82
 C      -3.771441    -1.612023    -0.469711      50.47
 H      -4.621606    -0.888566    -0.735363      20.39
 O      -3.139960    -2.249438    -1.584902     225.01
 H      -3.303512    -3.324299    -1.526446      16.49
 C      -4.210012    -2.471858     0.900623      65.53
 H      -3.416569    -2.758751     1.665836      20.31
 O      -5.004469    -1.542934     1.707831     319.78
 H      -4.267596    -1.058017     2.450401      19.19
 C      -5.147019    -3.675786     0.349479      89.08
 O      -4.795734    -4.624001    -0.650809     338.28
 H      -4.108006    -5.174198    -0.256396      29.47
 H      -6.100099    -3.158531     0.054628      27.93
 H      -5.350662    -4.256091     1.377821      25.86
55
name = lig-etoh-frame_545
 C       2.240472     1.604247    -1.791518      78.79
 H       1.773904     2.270520    -2.447020      21.55
 C       3.203763     1.311421     0.410820      19.10
 H       3.159530     1.750427     1.429635      21.23
 C       3.892848     0.116408    -0.145143      51.91
 O       4.558871    -0.919018     0.734669     257.80
 C       5.979379    -0.388254     0.958922      88.25
 H       6.562152    -0.631893     0.104726      25.80
 H       6.338637    -1.008063     1.703180      26.77
 H       5.781925     0.806644     1.275022      22.42
 C       3.577758    -0.309867    -1.384551      18.48
 O       4.141739    -1.481728    -1.859738     162.05
 H       4.993588    -1.792117    -1.126952      19.13
 C       2.660889     0.346978    -2.227930      42.91
 H       2.547823     0.175602    -3.309319      22.20
 C       2.611593     2.165255    -0.490206      46.44
 C       1.942366     3.595602    -0.045782      94.91
 H       2.011135     4.272416    -0.831911      20.06
 O       2.468112     4.166147     1.098813     310.67
 H       3.455528     4.193026     1.039575      27.00
 C       0.200892     3.581991    -0.048520      36.50
 H      -0.176741     3.284942    -1.100827      16.58
 C      -0.332009     5.134853     0.560816      97.58
 O       0.225877     6.186902    -0.366623     264.31
 H       0.499183     5.789291    -1.197479      31.38
 H       0.186598     5.388315     1.403781      25.00
 H      -1.373256     5.164305     0.575960      24.97
 C      -1.409277    -0.876707     0.429427      29.46
 H      -1.206558    -1.881525     0.386744      13.97
 C      -3.552530     0.777657     0.075693      36.01
 H      -4.566570     0.823627    -0.115950      16.01
 C      -2.581717     1.878757     0.280817     -16.65
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 O      -2.917240     3.210029     0.679048     213.62
 C      -3.957288     3.750480    -0.210867      83.77
 H      -4.631532     2.951396    -0.508795      25.78
 H      -4.493968     4.405294     0.775626      21.42
 H      -3.336643     4.338135    -1.011736      23.53
 C      -1.144892     1.572851     0.332596      10.99
 O      -0.312692     2.534069     0.883586     200.21
 C      -0.619279     0.317574     0.311585      47.20
 H       0.353273     0.264916     0.548839      15.75
 C      -2.817730    -0.509188     0.017149      11.21
 C      -3.835908    -1.581529    -0.387011      65.16
 H      -4.613316    -1.076467    -0.961286      20.09
 O      -3.124549    -2.300037    -1.575526     250.04
 H      -3.363961    -3.175931    -1.520976      21.92
 C      -4.224829    -2.514258     0.836964      88.69
 H      -3.312877    -2.666963     1.421269      22.17
 O      -5.059197    -1.606099     1.732492     355.52
 H      -4.441736    -1.254184     2.412548      24.05
 C      -5.157079    -3.673835     0.469337      94.00
 O      -4.772596    -4.616351    -0.714465     277.01
 H      -4.059614    -5.294845    -0.268296      24.55
 H      -5.948315    -3.101316    -0.038168      28.76
 H      -5.509131    -4.199406     1.351892      27.57
55
name = lig-etoh-frame_546
 C       2.212509     1.587321    -1.841907      64.99
 H       1.609175     2.307357    -2.493855      18.53
 C       3.225354     1.312184     0.365038      41.08
 H       3.435790     1.380375     1.442820      21.88
 C       3.877567     0.134247    -0.120106      40.99
 O       4.614106    -0.877856     0.696775     281.40
 C       5.920200    -0.400493     0.999325      90.61
 H       6.579874    -0.395119     0.047232      24.82
 H       6.434889    -0.951053     1.923498      24.98
 H       5.815685     0.618831     1.078204      29.18
 C       3.614977    -0.355178    -1.441618      14.10
 O       4.121623    -1.446886    -1.854093     238.88
 H       4.767381    -1.765104    -1.384617      24.00
 C       2.665661     0.390686    -2.232482      51.25
 H       2.693493     0.174857    -3.359937      23.01
 C       2.587550     2.207736    -0.483308      62.30
 C       1.884569     3.589938    -0.047692      90.45
 H       2.217400     4.315875    -1.060828      17.84
 O       2.363967     4.159307     1.105674     286.45
 H       3.396910     3.922975     1.141071      23.09
 C       0.211284     3.595307    -0.061625      50.58
 H      -0.141448     3.232536    -0.982661      17.77
 C      -0.317166     5.183602     0.603075      73.16
 O       0.264658     6.142810    -0.403210     237.17
 H       0.332393     5.731187    -1.309989      28.33
 H       0.074476     5.203698     1.765052      21.85
 H      -1.468085     5.285931     0.549326      22.07
 C      -1.458113    -0.814184     0.385799      34.05
 H      -1.011374    -1.898148     0.232628      13.54
 C      -3.494475     0.877365     0.021004      56.63
 H      -4.650991     0.716376    -0.032939      18.05
 C      -2.559737     1.808581     0.211317       2.53
 O      -2.843418     3.183521     0.737334     154.59
 C      -4.017429     3.754389    -0.258919     109.78
 H      -4.751074     2.994657    -0.641608      26.08
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 H      -4.477230     4.417913     0.315579      28.09
 H      -3.677923     4.355836    -1.120145      26.97
 C      -1.180169     1.585400     0.343738       8.24
 O      -0.309635     2.583153     0.888785     172.70
 C      -0.589462     0.314163     0.339530      31.86
 H       0.545866     0.244740     0.819206      13.20
 C      -2.816870    -0.486289     0.102942      52.96
 C      -3.855498    -1.572146    -0.335241      65.51
 H      -4.810556    -1.418156    -0.955454      20.64
 O      -3.110941    -2.344566    -1.551006     172.76
 H      -3.578211    -3.300455    -1.487247      16.66
 C      -4.241096    -2.506720     0.780714     104.44
 H      -3.160136    -2.837394     1.087118      20.60
 O      -5.122836    -1.702076     1.721059     335.06
 H      -4.458950    -1.328563     2.500261      21.65
 C      -5.170444    -3.663925     0.537922      80.66
 O      -4.730640    -4.605429    -0.733573     245.80
 H      -4.109470    -5.237250    -0.433284      29.08
 H      -6.000448    -3.149758    -0.052081      27.47
 H      -5.753008    -4.298174     1.396976      26.09
55
name = lig-etoh-frame_547
 C       2.182933     1.681490    -1.818693      38.54
 H       1.532357     2.146319    -2.540875      15.86
 C       3.293273     1.291808     0.350055      69.55
 H       3.653365     1.265035     1.418083      18.37
 C       3.847543     0.110003    -0.102878      26.50
 O       4.638134    -0.813665     0.647642     299.25
 C       5.904087    -0.409654     1.014940     112.53
 H       6.583449    -0.391474     0.189484      28.44
 H       6.307937    -0.778993     1.876646      29.58
 H       5.927915     0.833440     1.231751      27.68
 C       3.608428    -0.311508    -1.437606      10.66
 O       4.107184    -1.475775    -1.917160     160.76
 H       4.933970    -1.912753    -1.280036      17.54
 C       2.718987     0.408405    -2.271007      48.70
 H       2.655124    -0.014633    -3.381683      23.92
 C       2.488219     2.226581    -0.519399     104.21
 C       1.809512     3.566550    -0.141886     125.66
 H       2.174098     4.172748    -0.913849      25.07
 O       2.269010     4.134632     1.144454     330.63
 H       3.210897     3.999512     1.173301      29.13
 C       0.238391     3.636944     0.004727      65.32
 H      -0.164053     3.454290    -1.083978      15.81
 C      -0.271644     5.169324     0.566743      99.04
 O       0.310930     6.110138    -0.390240     271.48
 H      -0.111929     5.639433    -1.281262      25.85
 H      -0.099386     5.160221     1.558462      26.19
 H      -1.383807     5.275765     0.565063      23.59
 C      -1.521860    -0.735721     0.286565      58.01
 H      -1.017041    -1.682552     0.221529      16.16
 C      -3.404229     0.837170    -0.029491      78.35
 H      -4.492601     0.973414     0.087492      27.27
 C      -2.518214     1.867498     0.200413       9.09
 O      -2.823024     3.142784     0.717241     141.42
 C      -4.051444     3.741566    -0.281523      90.82
 H      -4.737447     2.992652    -0.640417      26.93
 H      -4.752567     4.704350     0.244174      23.18
 H      -3.752584     4.250181    -1.180952      26.65
 C      -1.156661     1.600812     0.378602      -1.63
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 O      -0.307342     2.634521     0.887896     211.19
 C      -0.550476     0.290022     0.420470      24.51
 H       0.390079     0.286892     0.715250      16.67
 C      -2.901204    -0.466135     0.148078      66.76
 C      -3.854051    -1.601161    -0.358748      68.72
 H      -4.839544    -1.301578    -0.686267      23.52
 O      -3.109761    -2.401855    -1.495696     206.28
 H      -3.749745    -3.230619    -1.520415      16.49
 C      -4.230099    -2.510070     0.778449     120.68
 H      -3.331363    -3.007041     1.106671      22.14
 O      -5.150304    -1.807848     1.707231     353.81
 H      -4.541436    -1.358840     2.469307      21.56
 C      -5.223749    -3.685034     0.507587      94.51
 O      -4.700244    -4.571613    -0.718470     271.06
 H      -3.982686    -5.230553    -0.426303      26.57
 H      -6.135932    -3.286452     0.088494      29.67
 H      -5.562878    -4.228586     1.312701      28.95
55
name = lig-etoh-frame_548
 C       2.174547     1.744726    -1.798891      43.81
 H       1.476664     2.163261    -2.532867      15.47
 C       3.353688     1.300917     0.349700     121.36
 H       3.603168     1.649987     1.354471      13.32
 C       3.820582     0.068396    -0.124943      -0.87
 O       4.621960    -0.755960     0.603443     284.21
 C       5.927488    -0.309920     1.016030     101.39
 H       6.714199    -0.611252     0.231724      26.07
 H       6.177832    -0.947860     2.010148      25.70
 H       5.948059     0.654704     1.394772      30.71
 C       3.582157    -0.263367    -1.434265      18.79
 O       4.119896    -1.540472    -1.992203     177.41
 H       4.838092    -1.850615    -1.283631      19.38
 C       2.780737     0.446296    -2.303143      39.08
 H       2.525369    -0.020138    -3.240608      23.54
 C       2.385619     2.180653    -0.536379     124.24
 C       1.737868     3.529075    -0.180692     117.46
 H       2.082716     4.428119    -1.029108      26.20
 O       2.174989     4.086612     1.178097     242.73
 H       3.198581     4.218033     1.157005      29.69
 C       0.236236     3.700725     0.048575      97.16
 H      -0.199930     3.682675    -0.883126      20.60
 C      -0.222333     5.090843     0.468734     106.83
 O       0.338007     6.074553    -0.359113     285.10
 H      -0.132839     5.899088    -1.141728      34.23
 H       0.104559     5.359820     1.615550      24.98
 H      -1.348658     5.117973     0.434885      24.85
 C      -1.550448    -0.662547     0.188167      58.86
 H      -1.234611    -1.743815     0.222929      17.92
 C      -3.328397     0.791809    -0.046477      75.87
 H      -4.371385     1.193276     0.048904      23.50
 C      -2.448081     1.962208     0.228713       0.21
 O      -2.878820     3.135615     0.631706     193.87
 C      -4.093444     3.757188    -0.249604      97.19
 H      -4.709223     2.847995    -0.452583      25.06
 H      -4.662366     4.493988     0.209616      25.60
 H      -3.450012     4.067273    -1.204863      24.52
 C      -1.061761     1.620339     0.430232      11.12
 O      -0.301363     2.677370     0.891690     221.97
 C      -0.607488     0.314421     0.493684      30.24
 H       0.605130     0.199527     0.605191      14.77
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 C      -2.998746    -0.490585     0.116914      43.08
 C      -3.829977    -1.644954    -0.399322      61.17
 H      -4.752348    -0.954397    -0.616522      20.00
 O      -3.139830    -2.444493    -1.418298     263.50
 H      -3.728247    -3.175180    -1.549465      18.82
 C      -4.257198    -2.564622     0.805946      98.31
 H      -3.434231    -3.088603     1.474504      16.96
 O      -5.142688    -1.898756     1.705164     383.97
 H      -4.655981    -1.428535     2.333715      29.90
 C      -5.254636    -3.715142     0.383800      70.52
 O      -4.684592    -4.532404    -0.680390     322.10
 H      -3.856245    -5.053559    -0.269787      23.37
 H      -6.349965    -3.376396     0.169005      27.15
 H      -5.170709    -4.354567     1.470819      26.00
55
name = lig-etoh-frame_549
 C       2.180280     1.713308    -1.849486      44.88
 H       1.479802     2.370619    -2.456876      15.73
 C       3.347075     1.371083     0.326758      80.24
 H       3.519132     2.039150     1.210592      13.16
 C       3.800756     0.090188    -0.130128      11.97
 O       4.609368    -0.721919     0.576897     262.45
 C       5.970474    -0.266037     1.048704      99.32
 H       6.683911    -0.617681     0.326382      27.33
 H       5.968313    -1.003833     1.781756      27.41
 H       5.870425     0.849586     1.322066      27.35
 C       3.568799    -0.305649    -1.508307      17.17
 O       4.120524    -1.566761    -2.043380     201.25
 H       4.729356    -1.844130    -1.395375      24.51
 C       2.814390     0.549014    -2.298808      50.85
 H       2.299431     0.012989    -3.290452      21.19
 C       2.333480     2.108461    -0.493299      91.45
 C       1.710395     3.552847    -0.164819     106.51
 H       1.881475     4.273513    -0.865248      24.43
 O       2.116099     4.018280     1.196964     270.55
 H       3.030668     4.467333     1.066446      27.73
 C       0.218621     3.728891     0.046532      81.58
 H      -0.399967     3.588403    -0.955156      18.34
 C      -0.179003     5.023598     0.452386     119.18
 O       0.368560     6.069879    -0.320609     227.82
 H       0.058180     6.181110    -1.335553      28.91
 H       0.134227     5.408337     1.328908      26.22
 H      -1.311499     4.923930     0.329257      23.02
 C      -1.576536    -0.655087     0.124108      47.75
 H      -1.409335    -1.780064     0.173260      16.66
 C      -3.286576     0.874899    -0.024492      59.07
 H      -4.405426     1.201221    -0.185984      21.63
 C      -2.369252     1.936961     0.251347       2.04
 O      -2.980898     3.193685     0.540755     242.54
 C      -4.059490     3.697394    -0.234493     104.36
 H      -4.751672     2.873078    -0.347693      24.43
 H      -4.637457     4.602975     0.461549      23.05
 H      -3.490234     3.944327    -1.036941      26.98
 C      -0.997993     1.698257     0.484019      19.02
 O      -0.270369     2.722982     0.925188     240.10
 C      -0.643797     0.340107     0.540240      49.04
 H       0.356864     0.050479     0.425939      19.53
 C      -2.983571    -0.548231     0.029430      29.86
 C      -3.826199    -1.673881    -0.390047      71.50
 H      -4.647662    -1.136352    -0.837281      19.40
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 O      -3.172158    -2.458451    -1.344869     251.08
 H      -3.789899    -3.338884    -1.583741      14.70
 C      -4.321490    -2.641052     0.837762     103.23
 H      -3.522369    -2.960754     1.452047      19.61
 O      -5.144716    -1.973184     1.706269     380.32
 H      -4.545527    -1.289360     2.401760      21.83
 C      -5.244523    -3.775197     0.321422     106.60
 O      -4.665488    -4.510900    -0.649443     398.81
 H      -3.911503    -4.811432    -0.228818      31.34
 H      -6.238923    -3.511322     0.182196      28.29
 H      -5.137337    -4.343579     1.132178      28.55
55
name = lig-etoh-frame_550
 C       2.168037     1.696403    -1.869957      56.54
 H       1.620107     2.364925    -2.453318      19.59
 C       3.271179     1.478915     0.275149      35.22
 H       3.627264     2.021271     1.145233      16.63
 C       3.788515     0.163782    -0.165880      21.95
 O       4.612383    -0.707535     0.565375     265.79
 C       5.957599    -0.244797     1.073469      81.93
 H       6.689669    -0.346106     0.228360      26.88
 H       6.047850    -0.956002     1.969820      25.42
 H       5.868624     0.908265     1.104917      27.20
 C       3.572662    -0.371899    -1.571388       5.96
 O       4.088285    -1.543384    -2.090216     147.68
 H       4.838985    -1.981200    -1.297551      20.36
 C       2.797244     0.603997    -2.352285      62.34
 H       2.433097     0.287688    -3.232768      23.65
 C       2.317641     2.059648    -0.466259      41.81
 C       1.699748     3.538032    -0.079234     100.13
 H       2.022402     4.356470    -1.037445      19.22
 O       2.096302     3.956900     1.199460     290.70
 H       2.840496     4.497647     1.075746      28.46
 C       0.192351     3.650615    -0.050603     100.95
 H      -0.313414     3.369127    -0.913141      22.14
 C      -0.203794     5.027456     0.440802      98.81
 O       0.411053     6.116110    -0.306352     262.09
 H       0.329618     6.047622    -1.321872      29.56
 H       0.060637     5.256189     1.576366      23.44
 H      -1.286885     4.990244     0.421423      24.15
 C      -1.598966    -0.708154     0.109314      47.14
 H      -1.176330    -1.697940     0.064292      19.39
 C      -3.287815     0.939651    -0.004202      69.10
 H      -4.272208     1.111956    -0.314837      21.21
 C      -2.364601     1.893522     0.269599       2.72
 O      -3.031405     3.244841     0.493027     215.56
 C      -4.050916     3.636624    -0.198411     126.27
 H      -4.976409     3.012835    -0.417080      25.06
 H      -4.332524     4.515473     0.401516      24.75
 H      -3.805407     4.128381    -1.342770      24.37
 C      -0.991368     1.759748     0.541814      20.77
 O      -0.211128     2.776799     1.003470     242.77
 C      -0.686578     0.343179     0.529314      34.92
 H       0.386673    -0.027623     0.423698      19.88
 C      -2.906009    -0.502155    -0.080216      44.39
 C      -3.870897    -1.706435    -0.350187      68.71
 H      -4.820798    -1.485093    -1.012817      16.84
 O      -3.182555    -2.499054    -1.315412     291.82
 H      -3.727134    -3.239281    -1.412688      19.23
 C      -4.388888    -2.669186     0.828291      88.75
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 H      -3.308918    -3.041743     1.224919      17.80
 O      -5.163066    -1.993296     1.756373     444.01
 H      -4.580045    -1.451108     2.218103      29.22
 C      -5.215062    -3.808924     0.341831      75.05
 O      -4.631638    -4.530031    -0.692381     340.19
 H      -3.700902    -4.869584    -0.285182      24.97
 H      -6.315142    -3.481042     0.021260      24.87
 H      -5.474502    -4.661061     1.296027      24.27
55
name = lig-etoh-frame_551
 C       2.143865     1.712249    -1.818628      62.54
 H       1.637808     2.365883    -2.646323      19.74
 C       3.238204     1.508766     0.247215      32.63
 H       3.738716     1.810844     1.182798      16.15
 C       3.795340     0.226589    -0.257890      36.48
 O       4.619166    -0.694887     0.564356     275.75
 C       5.905251    -0.226463     1.054661     117.66
 H       6.664819    -0.216274     0.253427      26.57
 H       6.343310    -0.558194     2.018019      27.54
 H       5.889763     0.854637     1.239098      30.27
 C       3.557052    -0.349530    -1.573974      19.76
 O       4.068817    -1.518366    -2.110097     239.65
 H       4.625408    -1.872191    -1.513439      29.96
 C       2.792538     0.566683    -2.413925      64.27
 H       2.667697     0.472256    -3.696935      20.01
 C       2.263617     2.110465    -0.508561      33.07
 C       1.722342     3.499636    -0.065125     137.12
 H       2.163817     4.115902    -0.735098      24.67
 O       2.098800     3.901743     1.209578     271.46
 H       2.922677     4.509265     1.149057      25.65
 C       0.191216     3.569835    -0.134125      75.67
 H      -0.244227     3.166829    -1.134988      20.70
 C      -0.248086     5.075941     0.437587      81.95
 O       0.460226     6.174795    -0.283780     262.71
 H       0.391335     5.743008    -1.172690      30.81
 H      -0.038951     4.869605     1.489300      24.75
 H      -1.409146     5.276399     0.444917      22.64
 C      -1.546103    -0.757785     0.133838      37.59
 H      -0.859655    -1.677065    -0.093643      13.71
 C      -3.293971     0.892084    -0.006574      25.43
 H      -4.416835     1.190745    -0.407719      12.23
 C      -2.422108     1.943696     0.299852      22.69
 O      -2.974711     3.232999     0.489179     241.24
 C      -4.124945     3.642997    -0.275652     132.59
 H      -5.063220     3.087003    -0.298009      26.42
 H      -4.423511     4.699754     0.378944      24.69
 H      -4.156728     4.016103    -1.202961      30.10
 C      -1.023945     1.736628     0.617119      -1.95
 O      -0.162762     2.803184     1.098709     220.76
 C      -0.697834     0.343783     0.470081      35.54
 H       0.412575     0.088209     0.676805      14.48
 C      -2.905813    -0.405746    -0.183184      50.11
 C      -3.958864    -1.722593    -0.355700      84.51
 H      -4.911691    -1.511029    -0.796226      23.58
 O      -3.149995    -2.542388    -1.305922     237.49
 H      -3.773727    -3.412651    -1.346422      12.33
 C      -4.382962    -2.667205     0.817657     104.64
 H      -3.469390    -3.141930     1.042353      25.24
 O      -5.192310    -2.005550     1.815675     411.94
 H      -4.474972    -1.389457     2.353684      22.98
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 C      -5.260129    -3.883897     0.420149     100.96
 O      -4.566284    -4.583232    -0.761500     323.36
 H      -3.728893    -5.075976    -0.513436      27.16
 H      -6.053305    -3.457260    -0.110802      30.77
 H      -5.642307    -4.452867     1.117069      29.61
55
name = lig-etoh-frame_552
 C       2.117564     1.703902    -1.852582      58.61
 H       1.642094     2.294593    -2.552615      19.53
 C       3.263507     1.433633     0.227110      36.54
 H       3.624167     1.698419     1.236603      15.97
 C       3.823588     0.265734    -0.338444      18.08
 O       4.614383    -0.676959     0.566352     263.25
 C       5.867022    -0.156125     1.005386     116.19
 H       6.652022    -0.326158     0.247473      25.53
 H       6.383516    -0.572923     1.898329      27.41
 H       5.712175     0.957684     1.397975      26.22
 C       3.517159    -0.259311    -1.584831      23.74
 O       4.033213    -1.475509    -2.137609     179.20
 H       4.703411    -1.929181    -1.404883      22.54
 C       2.778985     0.528550    -2.494108      47.00
 H       2.960719     0.531737    -3.443019      27.07
 C       2.222334     2.200639    -0.538062      52.59
 C       1.733451     3.439065    -0.088777     135.94
 H       2.442439     4.279134    -0.789914      19.85
 O       2.127405     3.858094     1.248283     242.86
 H       3.029365     4.313960     1.197514      27.13
 C       0.192008     3.551134    -0.166833      66.08
 H      -0.157085     3.078887    -1.072816      20.98
 C      -0.311133     5.100828     0.404466      82.50
 O       0.499717     6.212470    -0.242700     239.76
 H       0.450795     5.640257    -1.155629      27.11
 H       0.056748     4.865908     1.424858      24.34
 H      -1.294543     5.403907     0.288546      24.94
 C      -1.459037    -0.761624     0.140995      38.57
 H      -1.020973    -1.643892    -0.153106      15.63
 C      -3.350044     0.867370    -0.046994      43.51
 H      -4.266770     1.147731    -0.236949      16.34
 C      -2.474015     2.015143     0.345050      12.70
 O      -2.904824     3.220718     0.473028     177.04
 C      -4.253697     3.701614    -0.295489      82.96
 H      -5.031968     2.944237     0.040418      22.86
 H      -4.559332     4.660332     0.189468      25.37
 H      -4.062954     3.887880    -1.526747      22.95
 C      -1.106172     1.680616     0.703188      -3.93
 O      -0.156320     2.772585     1.153193     159.04
 C      -0.660162     0.356797     0.431479      46.56
 H       0.321803     0.227110     0.833120      15.33
 C      -2.928188    -0.425438    -0.245749      11.99
 C      -4.006297    -1.717003    -0.401842      65.84
 H      -5.035565    -1.230496    -0.737271      22.18
 O      -3.133043    -2.584913    -1.301674     211.44
 H      -3.603258    -3.498096    -1.357880      12.17
 C      -4.367821    -2.664070     0.829768      84.46
 H      -3.410655    -3.213406     1.291446      19.16
 O      -5.185239    -2.005671     1.875630     378.97
 H      -4.566943    -1.443022     2.550008      22.75
 C      -5.276847    -3.914498     0.398566      55.27
 O      -4.515219    -4.657534    -0.819257     260.33
 H      -3.831167    -5.281192    -0.493742      25.30
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 H      -6.070224    -3.420473    -0.298918      27.62
 H      -5.796961    -4.588196     1.375206      25.74
55
name = lig-etoh-frame_553
 C       2.103349     1.672930    -1.939700      89.19
 H       1.477683     2.393648    -2.603823      19.83
 C       3.258221     1.363630     0.190595      38.37
 H       3.398663     1.655268     1.220624      16.51
 C       3.871113     0.266474    -0.348294      28.38
 O       4.584157    -0.650259     0.549934     259.67
 C       5.854297    -0.051033     0.967634     104.71
 H       6.593622    -0.236252     0.135407      24.50
 H       6.056647    -0.888726     1.740630      24.41
 H       5.648795     0.915745     1.200691      31.17
 C       3.498526    -0.203998    -1.646437      28.78
 O       4.003957    -1.419546    -2.142848     160.07
 H       4.653391    -1.858289    -1.368164      21.76
 C       2.738721     0.555654    -2.475836      66.22
 H       3.148106     0.443411    -3.688940      22.35
 C       2.295083     2.154916    -0.562254      60.08
 C       1.759570     3.498716    -0.122454     122.86
 H       2.158853     4.208031    -0.731740      24.54
 O       2.172565     3.811687     1.291737     278.31
 H       3.089854     4.025638     1.199662      30.34
 C       0.196246     3.588530    -0.107263      55.18
 H      -0.254814     3.067866    -0.985181      20.59
 C      -0.310023     5.090083     0.347837      82.54
 O       0.525930     6.205039    -0.208469     211.49
 H       0.596317     6.118414    -1.152192      32.32
 H       0.031162     5.203750     1.451468      24.46
 H      -1.444005     5.341694     0.111458      23.45
 C      -1.448095    -0.709320     0.097906      30.97
 H      -1.196380    -1.845212    -0.142421      13.36
 C      -3.364819     0.886513    -0.083618      27.84
 H      -4.610900     1.114021    -0.130446      15.25
 C      -2.501227     1.967336     0.379148      15.89
 O      -2.887176     3.295804     0.440072     178.43
 C      -4.348753     3.720660    -0.315976      73.70
 H      -4.892907     2.920283     0.150769      23.62
 H      -4.636647     4.826447     0.129434      24.11
 H      -4.047815     3.514424    -1.247763      27.95
 C      -1.202071     1.655439     0.775905       1.02
 O      -0.192380     2.692225     1.145167     134.45
 C      -0.617711     0.374838     0.436330      45.64
 H       0.487681     0.257741     0.905867      13.13
 C      -2.913729    -0.532985    -0.241304       8.87
 C      -3.986710    -1.694564    -0.455294      69.37
 H      -4.851587    -1.178844    -0.836344      22.27
 O      -3.138202    -2.603367    -1.307673     238.69
 H      -3.503701    -3.515950    -1.315319      14.57
 C      -4.348778    -2.678969     0.889914      80.63
 H      -3.503218    -2.955576     1.416219      21.33
 O      -5.161229    -2.008470     1.921131     413.04
 H      -4.582277    -1.565934     2.547431      27.39
 C      -5.285079    -3.915894     0.318282      95.87
 O      -4.491306    -4.742138    -0.842984     272.16
 H      -3.945895    -5.460134    -0.246032      23.16
 H      -6.153419    -3.599649    -0.184818      30.23
 H      -5.516432    -4.480898     1.062501      30.92
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name = lig-etoh-frame_554
 C       2.075287     1.705584    -2.008238      70.55
 H       1.480080     2.350978    -2.616930      24.42
 C       3.209324     1.348274     0.160898      44.35
 H       3.257770     1.604518     1.248874      18.16
 C       3.901490     0.206358    -0.344870      51.56
 O       4.534491    -0.607305     0.498301     256.94
 C       5.840344    -0.030970     0.918357     102.34
 H       6.534032     0.024709     0.084708      25.10
 H       5.934840    -0.748761     1.673715      25.67
 H       5.733353     1.164996     1.204693      26.07
 C       3.538830    -0.197801    -1.672760      22.84
 O       3.986119    -1.364325    -2.136957     245.77
 H       4.476802    -1.676025    -1.475443      29.65
 C       2.714860     0.611891    -2.520628      58.37
 H       2.757377     0.340376    -3.463864      21.25
 C       2.404788     2.044349    -0.637291      40.78
 C       1.758327     3.545287    -0.096696      81.16
 H       1.953313     4.509954    -0.957514      15.92
 O       2.224566     3.767947     1.304729     236.63
 H       3.272264     3.792864     1.246871      25.49
 C       0.193346     3.630979     0.020152      58.91
 H      -0.383523     3.271183    -0.889275      19.18
 C      -0.282083     5.084361     0.278764     113.90
 O       0.549722     6.191999    -0.171576     196.32
 H       0.584293     6.497869    -1.138848      29.47
 H      -0.300507     5.343425     1.324354      26.56
 H      -1.284202     5.063051     0.034815      27.04
 C      -1.504339    -0.691723     0.010095      39.80
 H      -1.181955    -1.679593     0.037477      19.73
 C      -3.402702     0.867301    -0.109363      82.87
 H      -4.372132     0.944622    -0.107847      28.29
 C      -2.569925     1.893476     0.391734      -3.03
 O      -2.905070     3.403726     0.398840     133.52
 C      -4.372923     3.692414    -0.253416      80.76
 H      -5.096889     2.990664     0.183958      26.88
 H      -4.586077     4.889975    -0.199084      23.48
 H      -4.150325     3.272876    -1.348443      24.33
 C      -1.217653     1.646235     0.811364      -1.10
 O      -0.259850     2.600366     1.101793     170.40
 C      -0.589564     0.386272     0.495584      31.36
 H       0.389426     0.233396     0.677862      17.04
 C      -2.884033    -0.563916    -0.175835      32.43
 C      -3.869739    -1.692613    -0.472383      61.35
 H      -4.801605    -1.315810    -1.077602      19.85
 O      -3.155618    -2.596424    -1.332060     235.34
 H      -3.547662    -3.605468    -1.170355      12.54
 C      -4.380644    -2.657900     0.919992      57.86
 H      -3.305857    -2.896249     1.398379      15.37
 O      -5.149295    -2.024637     1.932371     321.70
 H      -4.339871    -1.568390     2.614895      18.88
 C      -5.217386    -3.886655     0.189585      76.09
 O      -4.494650    -4.831269    -0.812696     275.96
 H      -4.017989    -5.382173    -0.233845      27.15
 H      -6.314097    -3.643193    -0.126246      25.65
 H      -5.325230    -4.774584     1.135976      25.33
55
name = lig-etoh-frame_555
 C       2.067825     1.765390    -2.036945      78.66
 H       1.459177     2.414783    -2.676393      25.31
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 C       3.188937     1.309931     0.163549      46.19
 H       3.231531     1.552641     1.195860      20.06
 C       3.843130     0.186731    -0.382974      27.75
 O       4.518716    -0.585210     0.454943     277.14
 C       5.800854     0.009188     0.867715     102.68
 H       6.556500     0.067309     0.029940      25.50
 H       6.281518    -0.511312     1.826855      25.18
 H       5.734095     0.916197     1.263935      29.36
 C       3.578378    -0.151983    -1.671216      27.61
 O       3.975356    -1.337937    -2.166633     179.00
 H       4.605536    -1.805205    -1.292268      19.64
 C       2.710948     0.637628    -2.550733      56.62
 H       2.238486     0.147802    -3.666359      19.70
 C       2.424446     2.056898    -0.749963      24.78
 C       1.749608     3.556562    -0.072256      99.80
 H       1.930117     4.315823    -0.696850      22.20
 O       2.295646     3.733847     1.275540     271.80
 H       3.274925     3.714964     1.288695      28.61
 C       0.196478     3.634614     0.140287      76.06
 H      -0.269741     3.451556    -0.805300      19.18
 C      -0.252545     5.087345     0.246053     106.12
 O       0.582774     6.193326    -0.131034     198.30
 H       0.296664     6.477641    -1.084820      28.14
 H      -0.671918     5.316352     1.334671      25.27
 H      -1.308279     4.985536    -0.308667      22.96
 C      -1.525928    -0.666541    -0.037915      49.48
 H      -1.002523    -1.674828     0.058049      19.46
 C      -3.392730     0.793509    -0.104879      64.22
 H      -4.629612     0.906931    -0.236299      23.64
 C      -2.646102     1.880410     0.397297     -30.04
 O      -2.964653     3.469807     0.350447     154.47
 C      -4.319736     3.609849    -0.215274     117.31
 H      -5.282691     3.279921     0.309508      26.79
 H      -4.517108     4.799782    -0.365555      24.79
 H      -4.472921     3.331842    -1.241791      28.08
 C      -1.185898     1.622127     0.772340       4.29
 O      -0.318877     2.554853     1.068006     184.53
 C      -0.675337     0.366517     0.545350      27.88
 H       0.536497     0.175776     0.438398      17.36
 C      -2.884336    -0.499647    -0.103027      35.18
 C      -3.757643    -1.698875    -0.471991      86.55
 H      -4.635014    -1.462485    -1.052791      20.84
 O      -3.167255    -2.613294    -1.362597     288.38
 H      -3.491098    -3.435832    -1.191340      20.72
 C      -4.377148    -2.617710     0.883298      72.29
 H      -3.456899    -3.049669     1.122527      21.89
 O      -5.111790    -2.036692     1.942084     405.93
 H      -4.523590    -1.605654     2.443702      31.01
 C      -5.137871    -3.924700     0.151293     114.77
 O      -4.524349    -4.880489    -0.776826     348.10
 H      -3.826765    -5.424896    -0.196263      25.77
 H      -6.118545    -3.631936    -0.147284      28.90
 H      -5.270459    -4.521472     0.898443      29.65
55
name = lig-etoh-frame_556
 C       2.092883     1.810121    -2.084751      71.86
 H       1.426477     2.531971    -2.698389      21.33
 C       3.156477     1.288865     0.129746      43.41
 H       3.265508     1.551681     1.211518      17.33
 C       3.739923     0.237700    -0.399665      18.53
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 O       4.555989    -0.612573     0.446227     254.54
 C       5.792085     0.017633     0.838986     103.24
 H       6.473008    -0.015623     0.005644      26.56
 H       6.418918    -0.407157     1.560283      27.73
 H       5.472361     1.111851     1.279405      24.08
 C       3.569791    -0.095231    -1.750829      19.59
 O       4.004629    -1.359110    -2.183595     224.12
 H       4.496291    -1.830767    -1.534378      24.38
 C       2.690982     0.613192    -2.613398      56.78
 H       2.105599     0.155616    -3.272523      25.15
 C       2.380862     2.192988    -0.769239      32.35
 C       1.746804     3.468602    -0.007078     113.39
 H       2.171964     4.470506    -0.734663      17.66
 O       2.363548     3.705477     1.235248     267.43
 H       3.323881     3.820479     1.159788      29.53
 C       0.228440     3.593375     0.199682      77.06
 H      -0.064713     3.316131    -0.903969      18.11
 C      -0.329892     5.104271     0.279883     117.75
 O       0.607757     6.196105    -0.102021     203.21
 H       0.176359     6.264555    -0.909414      30.53
 H      -0.761103     5.259143     1.192470      28.10
 H      -0.964186     5.225775    -0.558755      25.99
 C      -1.482178    -0.651931    -0.009042      53.45
 H      -1.054589    -1.663387    -0.263056      17.93
 C      -3.454420     0.777896    -0.064460      60.91
 H      -4.410119     0.893724    -0.434844      24.70
 C      -2.656683     1.915320     0.406050     -30.33
 O      -3.046317     3.448085     0.298727     178.59
 C      -4.294047     3.568782    -0.182058     115.73
 H      -5.062128     3.458967     0.580455      26.84
 H      -4.332621     4.750789    -0.467273      23.94
 H      -4.593286     3.149509    -1.238468      25.61
 C      -1.232749     1.608793     0.665570       8.48
 O      -0.333795     2.587394     1.070113     204.40
 C      -0.748661     0.296511     0.540155      52.66
 H       0.236415     0.259064     0.425548      22.90
 C      -2.896829    -0.474327    -0.071430      22.61
 C      -3.714882    -1.703447    -0.437704      77.52
 H      -4.678789    -1.246944    -0.907996      19.58
 O      -3.132845    -2.624266    -1.404614     240.74
 H      -3.540362    -3.616114    -1.271788      11.36
 C      -4.330784    -2.598143     0.755393      65.74
 H      -3.405365    -3.264041     1.155332      16.68
 O      -5.088049    -2.068638     1.909945     301.40
 H      -4.414244    -1.377937     2.544905      19.15
 C      -5.074144    -3.937722     0.163391      74.77
 O      -4.537732    -4.914851    -0.741811     318.12
 H      -3.680558    -5.352780    -0.355454      25.51
 H      -6.003918    -3.574863    -0.410908      25.71
 H      -5.446533    -4.520452     1.291191      24.85
55
name = lig-etoh-frame_557
 C       2.132547     1.867645    -2.121216      35.23
 H       1.500272     2.444857    -2.685917      20.34
 C       3.064381     1.374771     0.090915      43.03
 H       3.276250     1.552304     1.133286      18.33
 C       3.699606     0.236725    -0.410115      15.67
 O       4.582188    -0.660683     0.434079     227.15
 C       5.780615     0.073128     0.804177      96.56
 H       6.389072     0.129663    -0.150305      26.80
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 H       6.326433    -0.642178     1.556026      25.30
 H       5.458866     1.035506     0.996789      29.19
 C       3.548782    -0.096345    -1.855891      15.17
 O       4.026891    -1.373684    -2.229487     186.09
 H       4.531536    -1.846283    -1.478115      21.28
 C       2.659111     0.616659    -2.620122      59.59
 H       2.015389    -0.062464    -3.445072      20.94
 C       2.326771     2.318040    -0.713319      26.21
 C       1.796270     3.422338     0.015974     135.74
 H       2.013106     4.194524    -0.575497      22.92
 O       2.439284     3.674301     1.222933     246.02
 H       3.382221     4.091009     0.947213      26.75
 C       0.259034     3.542155     0.151559      67.08
 H       0.010946     3.168207    -0.788320      20.61
 C      -0.391897     5.099764     0.308764      88.57
 O       0.629362     6.190258    -0.055729     146.60
 H       0.360038     6.289750    -1.054750      27.90
 H      -0.958510     5.344098     1.345664      24.24
 H      -1.066609     5.243111    -0.556694      24.18
 C      -1.502716    -0.724170     0.019050      42.78
 H      -1.152308    -1.593615    -0.492326      16.87
 C      -3.495103     0.832649     0.003999      65.11
 H      -4.535421     0.958912    -0.573598      19.26
 C      -2.636892     1.966254     0.390808       0.39
 O      -3.058539     3.331829     0.265377     230.08
 C      -4.342398     3.587532    -0.193135      91.96
 H      -4.920712     3.451710     0.774480      26.29
 H      -4.290127     4.781330    -0.513478      22.98
 H      -4.585771     2.812326    -0.945969      26.18
 C      -1.329052     1.645869     0.558624      20.76
 O      -0.337345     2.636942     1.095689     183.79
 C      -0.772795     0.305066     0.521417      22.12
 H       0.426217     0.281978     0.578615      18.82
 C      -2.879769    -0.514969    -0.075758       8.48
 C      -3.764987    -1.704260    -0.409810      75.18
 H      -4.617112    -1.123727    -0.755004      20.26
 O      -3.084409    -2.633719    -1.441870     234.62
 H      -3.569196    -3.509021    -1.440588      14.37
 C      -4.214425    -2.650959     0.651181      95.16
 H      -3.431616    -3.047643     1.210232      19.94
 O      -5.040810    -2.089510     1.850277     351.65
 H      -4.460590    -1.465667     2.318879      25.59
 C      -5.097145    -3.932372     0.240268     101.00
 O      -4.521006    -4.935691    -0.712155     351.50
 H      -3.719061    -5.347017    -0.347362      27.79
 H      -5.811644    -3.603413    -0.510247      28.11
 H      -5.508716    -4.226658     1.067244      29.80
55
name = lig-etoh-frame_558
 C       2.179243     1.922517    -2.099599      32.25
 H       1.426381     2.457219    -2.868632      18.08
 C       2.997864     1.450183     0.058851      31.32
 H       3.180458     1.652111     1.115372      17.32
 C       3.690125     0.209224    -0.459873       3.77
 O       4.560953    -0.689617     0.392832     245.60
 C       5.784373     0.089950     0.733526      97.15
 H       6.393286     0.276956    -0.135049      27.87
 H       6.102922    -0.536689     1.536947      26.72
 H       5.565998     1.206462     1.086309      25.64
 C       3.548549    -0.157143    -1.866522      -0.22
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 O       4.045000    -1.381904    -2.298287     154.91
 H       4.531943    -1.654359    -1.287672      17.77
 C       2.577606     0.628606    -2.633365      57.18
 H       2.341729     0.157901    -3.582039      23.71
 C       2.308753     2.304617    -0.711958      34.93
 C       1.807397     3.447623     0.040620     103.86
 H       1.826592     4.464135    -0.784718      17.71
 O       2.544441     3.661996     1.237124     269.89
 H       3.263396     4.242803     1.023686      28.54
 C       0.260506     3.514189     0.092019      52.49
 H      -0.159547     3.116061    -0.946216      17.05
 C      -0.423358     5.085666     0.318218      91.77
 O       0.624152     6.172786    -0.010934     172.08
 H       0.832116     6.319242    -0.985907      30.55
 H      -0.794255     5.312556     1.240632      27.87
 H      -1.398447     5.024689    -0.261975      24.49
 C      -1.554490    -0.812928     0.044232      40.48
 H      -1.082097    -1.722222    -0.554233      15.33
 C      -3.499055     0.863777     0.065788      44.34
 H      -4.512499     0.996915    -0.379635      12.89
 C      -2.693725     1.994227     0.323177      11.51
 O      -3.003443     3.198568     0.247476     229.02
 C      -4.420554     3.595362    -0.169180      97.86
 H      -5.052050     3.524557     0.702650      27.72
 H      -4.387557     4.668030    -0.723434      23.85
 H      -4.753548     2.776788    -0.788214      26.86
 C      -1.316654     1.688300     0.518083      14.04
 O      -0.362643     2.667167     1.119826     188.30
 C      -0.734204     0.391892     0.481686      23.29
 H       0.275260     0.276029     0.817279      16.86
 C      -2.899435    -0.533132    -0.087940      49.25
 C      -3.825841    -1.700326    -0.428309      66.57
 H      -4.783550    -1.276328    -0.885035      21.35
 O      -3.044928    -2.609684    -1.475668     214.36
 H      -3.608747    -3.404364    -1.542094      17.96
 C      -4.124100    -2.739444     0.643232      86.35
 H      -3.100987    -2.925689     1.211208      17.80
 O      -4.995962    -2.121132     1.735241     288.58
 H      -4.353183    -1.469795     2.278651      21.02
 C      -5.105033    -3.877624     0.230670      71.68
 O      -4.503926    -4.938618    -0.677892     300.22
 H      -3.728333    -5.493780    -0.091225      21.11
 H      -5.923130    -3.461580    -0.409996      27.94
 H      -5.736137    -4.298377     1.290854      25.92
55
name = lig-etoh-frame_559
 C       2.176554     1.946190    -2.116034      44.85
 H       1.591455     2.487731    -2.720906      20.05
 C       3.030717     1.395327     0.050410      25.74
 H       3.062254     1.741823     1.107253      14.87
 C       3.665697     0.207294    -0.515331       8.97
 O       4.511608    -0.669101     0.317524     241.76
 C       5.757241     0.122863     0.672435     106.95
 H       6.543481     0.195817    -0.110671      26.83
 H       6.232847    -0.412065     1.566076      26.67
 H       5.598890     1.032304     1.253726      26.62
 C       3.503687    -0.204674    -1.830324       7.80
 O       4.075855    -1.379117    -2.333238     240.58
 H       4.474031    -1.609855    -1.580531      26.39
 C       2.553272     0.661318    -2.603874      64.39
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 H       2.485155     0.494506    -3.818623      24.31
 C       2.302916     2.248201    -0.771289      39.08
 C       1.776009     3.576146    -0.000933     107.50
 H       1.901269     4.351973    -0.582631      24.92
 O       2.617060     3.665300     1.261421     252.96
 H       3.358236     4.357827     1.154801      28.36
 C       0.209798     3.520065     0.048672      81.72
 H      -0.132082     3.270162    -0.884925      22.80
 C      -0.403672     5.040619     0.277483      85.41
 O       0.593330     6.149166     0.039974     205.61
 H       0.986403     6.095824    -0.817016      32.95
 H      -0.444593     5.238426     1.491062      24.54
 H      -1.404981     4.988074    -0.121171      26.17
 C      -1.557101    -0.825543     0.067417      42.04
 H      -1.117382    -1.717522    -0.184589      16.36
 C      -3.480161     0.818430     0.112602      30.64
 H      -4.572927     0.966822    -0.092965      12.41
 C      -2.715625     1.882151     0.239917      19.79
 O      -2.998247     3.194664     0.222391     216.09
 C      -4.465709     3.564437    -0.138296     109.06
 H      -5.094139     3.625638     0.741337      27.45
 H      -4.454312     4.555588    -0.798410      25.07
 H      -5.024829     2.852426    -0.903310      26.20
 C      -1.219496     1.706056     0.539747      28.04
 O      -0.405627     2.683476     1.115157     227.49
 C      -0.747817     0.440232     0.417395      41.49
 H       0.254923     0.301345     0.937336      16.53
 C      -2.965732    -0.521819    -0.098924      31.67
 C      -3.871977    -1.710890    -0.504219      62.56
 H      -4.849793    -1.616521    -1.011180      20.49
 O      -3.021145    -2.553155    -1.503317     191.97
 H      -3.650141    -3.429354    -1.648724      17.06
 C      -4.061857    -2.799993     0.718300      95.81
 H      -3.046774    -3.056040     0.927051      23.38
 O      -4.933475    -2.143774     1.601994     376.38
 H      -4.373581    -1.584846     2.365055      23.00
 C      -5.113614    -3.855237     0.217012     100.67
 O      -4.493831    -4.930605    -0.615983     372.50
 H      -3.946273    -5.422317    -0.061668      31.93
 H      -5.963822    -3.285752    -0.223825      29.49
 H      -5.514504    -4.314155     1.020564      28.25
55
name = lig-etoh-frame_560
 C       2.153229     1.920733    -2.139703      64.57
 H       1.600378     2.758708    -2.782710      16.87
 C       3.086275     1.297721     0.036776      40.64
 H       3.143566     1.598689     1.050628      15.50
 C       3.643903     0.210268    -0.517448      18.89
 O       4.476914    -0.608081     0.232003     253.13
 C       5.732063     0.113657     0.663024     109.76
 H       6.521507     0.109029    -0.121681      25.88
 H       6.332311    -0.464437     1.390070      26.69
 H       5.408903     1.070623     1.129567      26.34
 C       3.393558    -0.212481    -1.836513      13.31
 O       4.089558    -1.349172    -2.376733     149.65
 H       4.728917    -1.919792    -1.583501      19.53
 C       2.592266     0.674626    -2.599236      83.88
 H       2.617621     0.860512    -3.694951      27.06
 C       2.306987     2.229443    -0.784445      42.46
 C       1.764869     3.625661    -0.041112      88.12
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 H       2.254323     4.662182    -0.689319      21.37
 O       2.632770     3.684537     1.277058     223.70
 H       3.466123     4.291852     1.164420      28.03
 C       0.161943     3.598142     0.058794      79.59
 H      -0.122536     3.232193    -1.032474      18.32
 C      -0.330639     4.982162     0.314587     116.04
 O       0.539896     6.120476     0.082342     204.20
 H       0.965355     5.808129    -0.798980      30.82
 H      -0.236832     4.947393     1.331692      26.66
 H      -1.334523     5.228547    -0.160114      24.34
 C      -1.580600    -0.716553     0.095049      44.73
 H      -1.118322    -1.827577     0.256459      14.50
 C      -3.513340     0.696878     0.116973      42.91
 H      -4.673830     0.899591     0.325840      14.15
 C      -2.601940     1.796131     0.192382       6.39
 O      -3.062783     3.243505     0.180241     183.98
 C      -4.491853     3.508512    -0.133262     100.42
 H      -4.917391     3.635714     0.913463      24.00
 H      -4.396857     4.596368    -0.732578      23.32
 H      -5.002682     2.909127    -0.807479      27.84
 C      -1.188994     1.699190     0.557179      13.26
 O      -0.441654     2.706954     1.078389     229.31
 C      -0.757989     0.391898     0.370147      46.76
 H       0.277065     0.255401     0.836566      16.68
 C      -3.011172    -0.545389    -0.115317      24.99
 C      -3.863655    -1.781594    -0.584699      64.97
 H      -4.866236    -1.649808    -1.028381      21.57
 O      -3.024329    -2.493580    -1.533933     278.31
 H      -3.423442    -3.303662    -1.682685      22.66
 C      -4.052405    -2.812742     0.717867      86.95
 H      -3.033383    -3.352126     0.911969      19.12
 O      -4.865134    -2.140613     1.532930     393.71
 H      -4.460549    -1.738302     2.247685      31.40
 C      -5.064721    -3.858744     0.189007      76.33
 O      -4.528250    -4.888347    -0.582107     314.03
 H      -3.872809    -5.476867     0.076413      24.23
 H      -5.881104    -3.283212    -0.256281      29.00
 H      -5.493726    -4.504413     1.230830      24.83
55
name = lig-etoh-frame_561
 C       2.099151     1.920907    -2.121276      48.16
 H       1.773816     2.692928    -2.783723      23.79
 C       3.079079     1.288700     0.016078      46.19
 H       3.382011     1.390221     1.115826      17.78
 C       3.633645     0.165023    -0.525378      24.63
 O       4.482887    -0.561204     0.167253     242.12
 C       5.704296     0.080689     0.660665     106.74
 H       6.297027     0.229284    -0.244181      26.18
 H       6.132568    -0.601974     1.390093      25.46
 H       5.349655     1.167582     0.852286      26.49
 C       3.304243    -0.232227    -1.862040      14.21
 O       4.098063    -1.311882    -2.411623     217.50
 H       4.600508    -1.829560    -1.764468      23.81
 C       2.656359     0.707068    -2.641663      54.52
 H       2.719283     0.676000    -3.777376      19.88
 C       2.321856     2.236120    -0.742016      28.13
 C       1.845105     3.633958    -0.089328     101.43
 H       2.189309     4.366355    -0.594984      22.66
 O       2.595904     3.712026     1.275107     258.82
 H       3.450911     4.081941     1.033620      28.48
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 C       0.164416     3.664792     0.016185      75.67
 H      -0.098227     3.213052    -0.879593      22.54
 C      -0.285129     4.964951     0.387073     108.64
 O       0.503864     6.085209     0.092842     235.17
 H       0.878901     5.849299    -0.798154      30.96
 H      -0.403321     4.809405     1.578955      23.47
 H      -1.199201     5.301845    -0.041142      24.02
 C      -1.619064    -0.638740     0.122682      48.69
 H      -1.316913    -1.538283     0.454215      16.78
 C      -3.569533     0.633357     0.122287      65.78
 H      -4.542097     0.781736     0.436085      16.42
 C      -2.507155     1.805326     0.182792       9.15
 O      -3.125896     3.242021     0.125297     178.64
 C      -4.471491     3.489750    -0.095215      93.95
 H      -4.930713     3.590558     0.857725      25.48
 H      -4.437880     4.614042    -0.575457      22.98
 H      -5.033752     2.649358    -0.768209      24.11
 C      -1.235429     1.659440     0.532281      13.69
 O      -0.451763     2.741754     1.019840     201.14
 C      -0.722842     0.320452     0.368384      51.96
 H       0.292191     0.083019     0.584145      18.03
 C      -3.026209    -0.629920    -0.145389       3.64
 C      -3.801214    -1.880817    -0.612627      65.71
 H      -4.813783    -1.441343    -0.929916      21.31
 O      -3.021591    -2.426145    -1.578880     269.00
 H      -3.305943    -3.412170    -1.706740      18.08
 C      -4.043808    -2.832938     0.598643     111.63
 H      -3.250597    -3.381021     1.131143      21.51
 O      -4.830775    -2.108279     1.525501     342.32
 H      -4.278171    -1.638115     2.425716      21.99
 C      -5.025501    -3.906737     0.242558     103.98
 O      -4.549347    -4.872560    -0.578892     381.04
 H      -3.852669    -5.375871    -0.129252      31.30
 H      -5.844771    -3.471816    -0.393351      28.56
 H      -5.458666    -4.227781     1.111209      28.28
55
name = lig-etoh-frame_562
 C       2.076862     1.907134    -2.068306      66.22
 H       1.739472     2.638199    -2.792217      24.21
 C       3.051913     1.325951     0.031487      36.95
 H       3.440548     1.398674     0.998762      19.46
 C       3.580827     0.124528    -0.584260      10.80
 O       4.517977    -0.578041     0.135702     258.54
 C       5.651835     0.078066     0.616858     115.61
 H       6.299118     0.244034    -0.281276      25.98
 H       5.924905    -0.573617     1.519696      24.75
 H       5.523633     1.076260     0.964414      28.20
 C       3.288072    -0.273219    -1.874003      13.98
 O       4.071638    -1.252692    -2.472381     199.89
 H       4.491830    -1.696429    -1.661957      22.58
 C       2.701802     0.767694    -2.723957      34.68
 H       2.719037     0.232452    -3.791969      19.72
 C       2.329097     2.255765    -0.693295      27.10
 C       1.923374     3.535929    -0.070489      79.09
 H       2.223635     4.528997    -0.924098      18.73
 O       2.516024     3.745289     1.240787     246.63
 H       3.523590     3.912083     0.975023      24.36
 C       0.242785     3.652803    -0.031760      54.46
 H      -0.176833     3.310159    -1.061366      20.76
 C      -0.300462     5.002343     0.510904     109.68
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 O       0.511195     6.074817     0.092090     243.82
 H       0.724844     6.065532    -0.828236      32.74
 H      -0.510028     5.057071     1.570146      26.38
 H      -1.380224     5.069136     0.098656      24.02
 C      -1.678232    -0.649027     0.136300      31.18
 H      -1.302674    -1.761161     0.426365      15.58
 C      -3.543036     0.627175     0.106431      67.70
 H      -4.744754     0.784724     0.417656      15.14
 C      -2.611354     1.849775     0.183864       9.75
 O      -3.113827     3.185135     0.075699     230.40
 C      -4.468687     3.452357    -0.070437     113.79
 H      -5.088603     3.394397     0.901074      25.21
 H      -4.683452     4.564878    -0.500341      23.90
 H      -4.922492     2.740968    -0.606855      28.19
 C      -1.210847     1.627209     0.492596       5.53
 O      -0.448297     2.763412     0.949531     189.71
 C      -0.678447     0.315595     0.399508      43.23
 H       0.443362    -0.101122     0.367537      17.15
 C      -3.031165    -0.667266    -0.156709      24.95
 C      -3.739371    -1.921046    -0.563281      95.10
 H      -4.672348    -1.477775    -0.857718      22.44
 O      -3.009355    -2.401331    -1.665670     263.04
 H      -3.174673    -3.444341    -1.685428      18.10
 C      -4.056693    -2.845364     0.502409     115.01
 H      -3.218169    -3.214654     1.152814      21.77
 O      -4.801202    -2.038082     1.575493     359.46
 H      -4.162613    -1.669173     2.119836      30.39
 C      -5.040766    -3.917666     0.272026      81.29
 O      -4.541492    -4.908711    -0.626574     332.69
 H      -3.736725    -5.427027    -0.249232      26.99
 H      -5.861276    -3.570194    -0.352448      26.95
 H      -5.597571    -4.201243     1.390138      24.67
55
name = lig-etoh-frame_563
 C       2.096978     1.875094    -2.059134      48.66
 H       1.469153     2.673908    -2.687184      21.51
 C       3.051097     1.312197     0.035804      34.17
 H       3.392680     1.630017     1.082257      18.17
 C       3.506097     0.133000    -0.608342      11.49
 O       4.525498    -0.640364     0.107332     256.77
 C       5.625692     0.090940     0.581496     131.86
 H       6.527080     0.062634    -0.049035      27.11
 H       5.996792    -0.452529     1.423098      27.76
 H       5.542942     1.075319     1.239807      25.11
 C       3.295844    -0.250975    -1.924958      17.95
 O       4.037113    -1.209267    -2.533727     159.71
 H       4.475587    -1.640954    -1.553550      18.10
 C       2.719094     0.771374    -2.761189      51.84
 H       2.542158     0.382894    -3.737186      21.68
 C       2.338125     2.242992    -0.678156      30.98
 C       1.944552     3.495059    -0.078574     107.49
 H       2.129960     4.166522    -0.733574      24.69
 O       2.439116     3.782195     1.178262     315.05
 H       3.406628     3.873328     1.198359      28.73
 C       0.330329     3.609533    -0.056560      60.09
 H      -0.073753     3.681789    -1.071951      21.03
 C      -0.346741     5.041594     0.573333      88.50
 O       0.535243     6.105539     0.099712     168.48
 H       0.384706     6.166086    -0.944524      28.74
 H      -0.361388     5.276928     1.737292      24.87
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 H      -1.344448     4.851233     0.227502      24.92
 C      -1.662775    -0.770797     0.164923      43.12
 H      -1.258439    -1.742146     0.007708      18.38
 C      -3.536765     0.686742     0.082494      43.63
 H      -4.515153     0.771404     0.101324      17.93
 C      -2.774995     1.840596     0.199209       1.80
 O      -3.052635     3.116982     0.038926     226.52
 C      -4.513042     3.411015    -0.014863     113.05
 H      -4.914661     3.125484     0.946973      28.10
 H      -4.720210     4.469732    -0.488412      24.07
 H      -5.012597     2.642343    -0.862942      24.59
 C      -1.165797     1.635750     0.440572       3.98
 O      -0.437222     2.751644     0.864893     206.74
 C      -0.664299     0.311647     0.420480      38.76
 H       0.305194     0.055943     0.381236      21.32
 C      -3.008672    -0.621165    -0.119253      16.55
 C      -3.703851    -1.880645    -0.531969      84.40
 H      -4.758394    -1.648604    -0.969709      19.93
 O      -2.997413    -2.423251    -1.757960     278.87
 H      -3.112850    -3.314629    -1.729190      22.90
 C      -4.081250    -2.850716     0.543325      94.18
 H      -3.032916    -3.132603     0.905006      21.06
 O      -4.778114    -1.974934     1.594481     311.10
 H      -3.947188    -1.507357     2.105433      20.05
 C      -5.106770    -3.946187     0.291286      87.93
 O      -4.521506    -4.971771    -0.687508     353.85
 H      -3.708979    -5.491817    -0.197985      25.49
 H      -6.003503    -3.486908    -0.202647      27.23
 H      -5.384973    -4.314559     1.246999      27.23
55
name = lig-etoh-frame_564
 C       2.113710     1.871178    -2.086812      38.63
 H       1.419960     2.474976    -2.511137      19.99
 C       3.074170     1.277827     0.058267      52.34
 H       3.287700     1.653269     1.026237      18.32
 C       3.475024     0.139681    -0.570474      10.44
 O       4.497680    -0.706966     0.063947     221.34
 C       5.655874     0.107414     0.608674     101.71
 H       6.613992     0.038601     0.034094      25.50
 H       6.105342    -0.602648     1.428719      25.30
 H       5.332911     1.001950     1.016375      28.30
 C       3.314574    -0.155774    -2.004000      32.26
 O       4.017051    -1.204330    -2.556627     239.26
 H       4.488533    -1.603780    -1.949093      27.84
 C       2.683746     0.764096    -2.739797      55.36
 H       2.257059     0.838286    -3.896187      18.90
 C       2.352358     2.162054    -0.722833      46.55
 C       1.871539     3.466380    -0.084156      94.83
 H       2.238929     4.420916    -0.956038      21.13
 O       2.368087     3.820569     1.158063     282.48
 H       3.319679     3.979686     1.276537      28.68
 C       0.382402     3.627579    -0.019362      80.95
 H       0.064555     3.755868    -1.046945      20.04
 C      -0.322136     5.049936     0.619830      92.02
 O       0.534167     6.160384     0.074447     185.24
 H       0.111227     6.206143    -0.795585      31.78
 H      -0.115395     5.203743     1.713922      25.76
 H      -1.391278     4.978633     0.265560      24.35
 C      -1.579739    -0.876522     0.177412      36.74
 H      -1.116650    -1.819808    -0.330393      15.47
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 C      -3.552561     0.740497     0.041635      17.07
 H      -4.752426     0.802640    -0.338739      16.16
 C      -2.781061     1.779391     0.233104      12.65
 O      -3.028610     3.092070     0.003285     218.27
 C      -4.560422     3.308451    -0.005967     107.35
 H      -4.846604     3.037533     1.021684      30.36
 H      -4.613604     4.533166    -0.281631      24.06
 H      -4.938603     2.837282    -0.794286      30.27
 C      -1.186124     1.630126     0.381821      14.70
 O      -0.418367     2.709600     0.767208     206.17
 C      -0.737374     0.306306     0.422947      27.94
 H       0.481562     0.232048     0.538278      17.72
 C      -2.944197    -0.563091    -0.047731      21.52
 C      -3.748503    -1.807112    -0.584662      70.44
 H      -4.674022    -1.642251    -1.033859      21.27
 O      -2.997206    -2.441007    -1.811664     209.35
 H      -3.189197    -3.495879    -1.762627      16.93
 C      -4.083101    -2.827666     0.649959      79.23
 H      -3.103985    -3.307552     0.849997      20.38
 O      -4.729910    -1.933274     1.587559     375.50
 H      -4.080701    -1.353181     2.241135      22.26
 C      -5.131380    -3.986752     0.253426      73.65
 O      -4.512206    -5.019323    -0.729954     346.78
 H      -3.906456    -5.489736    -0.153293      28.48
 H      -6.067870    -3.516164    -0.059786      27.08
 H      -5.314822    -4.641665     1.317918      25.13
55
name = lig-etoh-frame_565
 C       2.128750     1.882634    -2.078904      47.93
 H       1.253854     2.493114    -2.660721      16.80
 C       3.083607     1.260803     0.078944      59.66
 H       3.290871     1.482417     1.154890      17.44
 C       3.522279     0.087760    -0.547941       4.65
 O       4.469713    -0.755376     0.015824     235.92
 C       5.703909     0.045959     0.661037      49.97
 H       6.420436     0.249864    -0.177660      25.44
 H       5.925436    -0.563360     1.475379      24.88
 H       5.181268     1.090905     0.787554      22.26
 C       3.384214    -0.084899    -2.022019       5.73
 O       3.978463    -1.197419    -2.607527     132.57
 H       4.747564    -1.738490    -1.956005      19.11
 C       2.563032     0.813372    -2.786786      56.01
 H       2.354405     0.901957    -3.738731      28.36
 C       2.348005     2.099527    -0.770771      51.79
 C       1.817273     3.501070    -0.154084     120.58
 H       2.108518     4.206120    -0.730560      30.22
 O       2.307425     3.854266     1.191063     247.10
 H       3.310993     4.154047     1.068004      27.61
 C       0.347033     3.707280     0.022097      89.38
 H       0.047556     3.563371    -1.091353      21.76
 C      -0.209975     5.031789     0.631163     108.50
 O       0.494121     6.216578     0.042060     200.10
 H       0.081276     6.352284    -0.812780      30.76
 H      -0.130549     4.936978     1.722312      26.70
 H      -1.261275     5.254596     0.412444      25.54
 C      -1.488355    -0.912092     0.169928      36.98
 H      -1.072697    -1.773849    -0.409527      15.19
 C      -3.634256     0.700756    -0.027084      31.49
 H      -4.469539     0.825592    -0.530434      13.30
 C      -2.624798     1.782796     0.258463       3.45
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 O      -3.059457     3.090339    -0.027649     188.08
 C      -4.532045     3.257892     0.021794      95.25
 H      -5.000315     2.997608     1.005785      28.83
 H      -4.603457     4.417088    -0.004551      24.90
 H      -5.111708     2.756596    -0.945049      24.32
 C      -1.281019     1.587076     0.331471      18.65
 O      -0.396238     2.645454     0.683729     215.39
 C      -0.766347     0.287319     0.418610      33.56
 H       0.205294     0.317879     0.671464      20.19
 C      -2.885563    -0.570383    -0.002528       1.63
 C      -3.784830    -1.757386    -0.647207      41.68
 H      -4.794512    -1.346458    -1.108139      21.30
 O      -3.025375    -2.470853    -1.809022     224.85
 H      -3.348523    -3.433018    -1.757759      18.06
 C      -4.085437    -2.781891     0.710879      64.70
 H      -3.230964    -3.475895     1.083259      17.53
 O      -4.690895    -1.909694     1.577728     367.97
 H      -4.185179    -1.471722     2.353327      24.84
 C      -5.110196    -4.047030     0.248090      96.11
 O      -4.535619    -5.016911    -0.764676     314.66
 H      -3.959558    -5.658357    -0.078968      22.55
 H      -6.113082    -3.701356    -0.073030      29.02
 H      -5.278391    -4.763946     1.055004      27.29
55
name = lig-etoh-frame_566
 C       2.061761     1.938553    -2.106905      54.31
 H       1.482248     2.565867    -2.622772      20.84
 C       3.081429     1.234687     0.084408      45.00
 H       3.229357     1.297058     1.175257      18.31
 C       3.605796     0.039673    -0.581380       9.17
 O       4.470715    -0.804190    -0.012316     249.46
 C       5.679295    -0.004231     0.655817      63.03
 H       6.279510     0.227986    -0.214546      26.10
 H       5.925209    -0.493535     1.667775      23.82
 H       5.301515     0.964382     0.883997      26.84
 C       3.455537    -0.041559    -2.012075      -0.71
 O       3.952648    -1.200309    -2.664266     183.20
 H       4.631280    -1.507014    -1.983780      22.13
 C       2.487081     0.818844    -2.806549      37.05
 H       2.479484     0.632312    -4.067764      22.68
 C       2.320991     2.122310    -0.718712      33.61
 C       1.774120     3.499720    -0.160197      98.46
 H       2.179110     4.483129    -0.981849      22.03
 O       2.287892     3.883271     1.222439     251.17
 H       3.111454     4.254453     0.959027      29.28
 C       0.227254     3.747792    -0.036692      95.51
 H      -0.130310     3.614802    -1.000222      23.02
 C      -0.082644     5.033941     0.608739     109.24
 O       0.453602     6.267947     0.031856     181.87
 H       0.116675     6.407615    -0.941050      28.31
 H      -0.037830     4.808186     1.776036      24.59
 H      -1.158114     5.245488     0.526321      24.76
 C      -1.452000    -0.870306     0.148037      42.84
 H      -1.029114    -1.822047    -0.189914      16.33
 C      -3.542070     0.629034    -0.051038      71.57
 H      -4.553368     0.846915    -0.734370      15.05
 C      -2.600292     1.805131     0.215264      15.06
 O      -3.109287     3.088971    -0.042406     237.80
 C      -4.493102     3.216034     0.025894     118.18
 H      -5.042565     2.776062     0.878232      30.33
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 H      -4.691280     4.435067     0.219685      24.58
 H      -5.086211     2.888203    -0.742536      28.53
 C      -1.310359     1.551373     0.309272      25.83
 O      -0.371533     2.567115     0.644997     181.62
 C      -0.771070     0.254257     0.411407      32.51
 H       0.360267     0.264155     0.765478      17.67
 C      -2.897652    -0.635280    -0.040622      11.80
 C      -3.786994    -1.738630    -0.681225      56.34
 H      -4.649580    -1.226304    -0.969384      24.24
 O      -3.101628    -2.491145    -1.744702     279.37
 H      -3.492688    -3.337866    -1.731046      21.35
 C      -4.105528    -2.773887     0.690970      64.00
 H      -3.277433    -3.226413     1.226281      19.26
 O      -4.690512    -1.887966     1.569697     319.35
 H      -4.126859    -1.800462     2.537500      20.78
 C      -5.074971    -4.093748     0.236042      88.44
 O      -4.557635    -4.996624    -0.779006     353.11
 H      -3.987860    -5.635098    -0.413964      29.62
 H      -6.062088    -3.844636    -0.190256      27.30
 H      -5.325937    -4.821274     1.230329      25.47
55
name = lig-etoh-frame_567
 C       1.991007     1.974474    -2.133571      48.97
 H       1.517974     2.957430    -2.675227      17.44
 C       3.065434     1.178738     0.051583      32.14
 H       3.137448     1.268599     1.123560      18.79
 C       3.662386     0.074187    -0.656064      18.15
 O       4.515905    -0.862979    -0.000782     272.14
 C       5.601561    -0.062826     0.640090      96.33
 H       6.473805    -0.057708    -0.083143      25.35
 H       6.100454    -0.493764     1.504397      27.34
 H       5.296758     0.948817     1.111084      25.15
 C       3.463753    -0.018312    -2.042907      11.43
 O       3.930481    -1.178980    -2.712781     197.38
 H       4.568119    -1.494048    -2.017005      23.10
 C       2.499047     0.771989    -2.816086      40.97
 H       2.477602     0.464789    -3.746311      25.39
 C       2.280898     2.189844    -0.632946      42.58
 C       1.750255     3.543299    -0.160359     102.68
 H       2.043199     4.194743    -0.793651      27.04
 O       2.274071     3.898793     1.217477     243.18
 H       3.156656     4.369962     1.054891      26.09
 C       0.128880     3.700518    -0.158950      64.34
 H      -0.460983     3.839121    -1.187641      19.45
 C      -0.037367     5.064110     0.607595     105.17
 O       0.433323     6.319140     0.030706     219.29
 H       0.216814     6.189983    -0.911313      31.99
 H       0.312630     5.036191     1.581379      26.52
 H      -1.157114     5.015790     0.613040      24.71
 C      -1.504042    -0.840067     0.103560      49.44
 H      -0.989475    -1.909380     0.332823      18.18
 C      -3.376802     0.591375    -0.084848      33.98
 H      -4.345364     0.698666    -0.479253      23.14
 C      -2.730759     1.791111     0.111626       1.37
 O      -3.131894     3.081310    -0.046996     245.33
 C      -4.500717     3.224448     0.076628     112.30
 H      -4.847017     2.461907     0.850409      27.21
 H      -4.640488     4.308967     0.210347      24.70
 H      -5.102068     2.952205    -0.992097      24.69
 C      -1.238202     1.551335     0.316500       8.79
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 O      -0.333698     2.504076     0.648924     166.78
 C      -0.699902     0.247141     0.422001      38.18
 H       0.348216     0.134035     0.645190      20.76
 C      -2.916983    -0.717134    -0.144368      39.27
 C      -3.746554    -1.773074    -0.636491      73.18
 H      -4.765016    -1.258653    -0.945609      21.28
 O      -3.200246    -2.496187    -1.652023     236.54
 H      -3.737472    -3.452804    -1.727686      14.94
 C      -4.145181    -2.788795     0.608219      66.65
 H      -3.076267    -2.957440     1.079062      17.37
 O      -4.726050    -1.877342     1.583882     429.27
 H      -4.240066    -1.895262     2.308710      29.78
 C      -5.043811    -4.144340     0.258373      90.10
 O      -4.577675    -4.962512    -0.812255     354.07
 H      -3.818397    -5.609216    -0.539582      25.90
 H      -5.972339    -3.770886    -0.207328      27.27
 H      -5.292795    -4.507714     1.264911      26.09
55
name = lig-etoh-frame_568
 C       1.953706     1.995800    -2.124641      72.50
 H       1.631420     2.867734    -2.611462      22.16
 C       3.019329     1.147948    -0.006151      32.25
 H       3.137926     1.259713     1.116498      18.43
 C       3.700283     0.148187    -0.718005      11.40
 O       4.562188    -0.895025     0.020070     245.32
 C       5.564096    -0.129637     0.628320     119.18
 H       6.491867    -0.130567     0.075518      25.42
 H       6.063609    -0.817343     1.409412      26.05
 H       5.276933     0.844042     1.076760      27.51
 C       3.424285    -0.032104    -2.102455      21.35
 O       3.916936    -1.136934    -2.752867     144.60
 H       4.592379    -1.775488    -2.066411      20.36
 C       2.539677     0.779172    -2.727925      50.84
 H       2.295031     0.374582    -3.897454      19.65
 C       2.244328     2.213786    -0.632898      50.71
 C       1.708085     3.540992    -0.117670      88.65
 H       2.176598     4.420847    -1.013812      19.12
 O       2.257667     3.911415     1.184873     237.07
 H       3.190462     4.336896     1.184679      23.92
 C       0.086927     3.642397    -0.265271      83.51
 H      -0.530379     3.734211    -1.072251      22.46
 C      -0.086267     5.081230     0.605554      89.13
 O       0.412987     6.346341     0.012257     202.58
 H       0.391956     6.105260    -0.949031      31.20
 H       0.664915     5.073936     1.443045      23.66
 H      -1.150649     5.034587     0.862825      25.51
 C      -1.556360    -0.876516     0.098196      52.94
 H      -1.175123    -1.721140     0.544085      19.46
 C      -3.276427     0.563993    -0.144177      37.09
 H      -4.482101     0.587491    -0.290537      19.44
 C      -2.716208     1.745518     0.012255      16.65
 O      -3.122914     3.068603    -0.051560     248.84
 C      -4.572286     3.200003     0.087382     106.76
 H      -4.800432     2.474118     0.806186      27.98
 H      -4.679858     4.446073     0.388695      22.74
 H      -4.889266     3.102646    -0.885546      27.18
 C      -1.206686     1.559713     0.324314      -0.03
 O      -0.277912     2.500474     0.665965     160.89
 C      -0.654519     0.255195     0.412737      33.66
 H       0.436797     0.043984     0.560583      19.03
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 C      -2.842465    -0.758258    -0.240479      35.56
 C      -3.816009    -1.843580    -0.540140     101.67
 H      -4.730493    -1.463530    -0.891632      22.88
 O      -3.287926    -2.547977    -1.602778     303.55
 H      -3.816361    -3.319586    -1.698539      21.21
 C      -4.139796    -2.779011     0.530157      88.31
 H      -3.130669    -3.031399     0.739385      22.29
 O      -4.810633    -1.896103     1.554765     333.70
 H      -4.129134    -1.806576     2.454500      21.49
 C      -5.012092    -4.103533     0.274536      78.96
 O      -4.580230    -4.949286    -0.849789     356.22
 H      -3.689115    -5.384654    -0.484408      26.36
 H      -5.950931    -3.618436    -0.062813      26.67
 H      -5.252387    -4.562729     1.371859      25.03
55
name = lig-etoh-frame_569
 C       1.986885     1.963983    -2.044641      48.72
 H       1.523760     2.762851    -2.743277      23.57
 C       2.960952     1.168765    -0.044588      45.69
 H       3.190580     1.205047     0.982415      20.67
 C       3.731745     0.190809    -0.752756      17.23
 O       4.551160    -0.881853    -0.002320     237.77
 C       5.610675    -0.235000     0.667088      93.31
 H       6.456061     0.078857    -0.074458      23.68
 H       5.727825    -1.018421     1.435150      25.07
 H       5.271035     0.742532     1.046548      27.12
 C       3.407714    -0.088268    -2.106130      20.48
 O       3.927095    -1.125579    -2.795692     259.95
 H       4.334914    -1.670212    -2.264861      30.17
 C       2.524903     0.847495    -2.699726      57.62
 H       2.122149     0.652116    -3.623946      23.17
 C       2.215670     2.180973    -0.726138      36.94
 C       1.709302     3.565953    -0.158224     109.55
 H       2.050323     4.240608    -0.736178      25.96
 O       2.230271     3.917506     1.159392     288.51
 H       3.147075     4.145657     1.021840      25.86
 C       0.111686     3.627535    -0.239885      70.92
 H      -0.497336     3.444210    -1.258671      20.62
 C      -0.151190     5.073465     0.595148      92.91
 O       0.373298     6.348643    -0.032965     198.10
 H       0.604577     6.221294    -1.036587      28.33
 H       0.569230     4.683923     1.299559      25.09
 H      -1.100978     5.281598     1.155621      25.41
 C      -1.504119    -0.908097     0.142328      39.29
 H      -1.220159    -2.014989     0.608363      15.67
 C      -3.338247     0.524324    -0.256357      57.67
 H      -4.424989     0.550005    -0.047946      18.08
 C      -2.533184     1.739161    -0.056643      10.65
 O      -3.104165     3.044509    -0.048980     196.83
 C      -4.604529     3.226613     0.103431      95.10
 H      -5.127378     2.511988     0.891448      24.52
 H      -4.791217     4.180145     0.534303      25.86
 H      -5.080869     3.110547    -1.002407      23.17
 C      -1.193727     1.544064     0.317692      16.75
 O      -0.227759     2.546529     0.681308     171.78
 C      -0.677180     0.245894     0.371729      41.78
 H       0.446940     0.051515     0.546173      18.74
 C      -2.787051    -0.757473    -0.311831      22.90
 C      -3.927683    -1.882074    -0.491181      82.03
 H      -4.913956    -1.370503    -0.838514      21.43
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 O      -3.339779    -2.626322    -1.610271     253.15
 H      -3.936632    -3.448171    -1.755252      17.98
 C      -4.124234    -2.788880     0.541926      91.85
 H      -3.102305    -3.360991     0.794985      18.38
 O      -4.877899    -1.951093     1.532653     354.44
 H      -4.285293    -1.552904     2.242129      27.59
 C      -5.007409    -3.995460     0.290303      98.60
 O      -4.564820    -4.933505    -0.859050     370.87
 H      -3.775023    -5.242638    -0.504138      31.95
 H      -6.032428    -3.653342     0.095997      27.78
 H      -5.049870    -4.765689     1.133924      26.88
55
name = lig-etoh-frame_570
 C       2.025441     1.942701    -2.032728      50.75
 H       1.301430     2.483418    -2.703037      21.61
 C       2.940211     1.197881    -0.081265      52.45
 H       3.191381     1.270527     1.028123      19.74
 C       3.742169     0.182566    -0.754673      30.85
 O       4.482247    -0.827386    -0.077592     261.62
 C       5.675847    -0.329339     0.708983      95.36
 H       6.379970     0.028365     0.010275      25.20
 H       5.813576    -1.019995     1.535039      25.59
 H       5.288901     0.630833     1.249871      25.37
 C       3.387498    -0.111517    -2.081524      16.65
 O       3.927176    -1.115457    -2.873400     189.85
 H       4.358673    -1.810503    -2.098928      22.28
 C       2.506187     0.896908    -2.686452      52.06
 H       1.991080     0.817736    -3.773235      20.86
 C       2.200340     2.166442    -0.753311      42.21
 C       1.701199     3.535224    -0.207811      83.95
 H       2.163963     4.530441    -0.981252      20.18
 O       2.203140     3.907280     1.135003     258.12
 H       3.201896     3.952620     0.872140      23.45
 C       0.125212     3.647217    -0.180682      90.03
 H      -0.059458     3.309086    -1.163560      22.91
 C      -0.201054     5.041086     0.560865      96.50
 O       0.329707     6.330520    -0.076801     204.62
 H       0.613360     6.199924    -0.967501      31.48
 H       0.395155     4.694897     1.435159      24.41
 H      -1.041190     5.434588     1.134594      24.21
 C      -1.405669    -0.976311     0.211886      46.65
 H      -1.144394    -1.925885     0.334343      17.50
 C      -3.385625     0.541196    -0.361425      42.53
 H      -4.483994     0.639069    -0.099529      17.56
 C      -2.416810     1.725699    -0.114472      -0.41
 O      -3.095087     3.013949    -0.033078     165.24
 C      -4.618253     3.199470     0.093290      97.63
 H      -5.216724     2.578214     0.696711      26.94
 H      -4.796048     4.305389     0.724460      23.26
 H      -5.250145     3.165281    -0.786223      25.49
 C      -1.135136     1.547347     0.299664      23.31
 O      -0.209740     2.585452     0.703699     188.71
 C      -0.697509     0.191355     0.331092      49.02
 H       0.306066     0.157767     0.603158      20.71
 C      -2.820045    -0.754888    -0.347693       0.12
 C      -3.970830    -1.853916    -0.562536      58.70
 H      -4.903202    -1.337659    -0.687592      22.54
 O      -3.389903    -2.709276    -1.647302     220.14
 H      -3.971017    -3.598194    -1.823015      14.79
 C      -4.108691    -2.846450     0.663187     102.67
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 H      -3.256758    -3.275888     1.069894      22.84
 O      -4.936069    -2.019912     1.516879     404.12
 H      -4.365325    -1.425972     2.104168      27.96
 C      -5.033447    -3.940813     0.276712     100.05
 O      -4.567021    -4.884425    -0.857768     330.44
 H      -3.672822    -5.360718    -0.474706      24.22
 H      -6.116244    -3.765889     0.149758      28.17
 H      -4.912549    -4.730595     1.105149      27.19
55
name = lig-etoh-frame_571
 C       1.996211     1.953513    -2.112479      54.78
 H       1.187660     2.485322    -2.568963      19.42
 C       2.984833     1.216495    -0.071664      48.18
 H       3.098653     1.413494     0.965163      19.71
 C       3.706452     0.161213    -0.739364      33.77
 O       4.423422    -0.764779    -0.149220     223.15
 C       5.670913    -0.381129     0.762167      89.22
 H       6.599964    -0.201726     0.095786      22.68
 H       6.142977    -1.163451     1.480573      24.24
 H       5.418177     0.426371     1.393243      26.81
 C       3.350878    -0.082491    -2.101199      27.90
 O       3.931356    -1.122143    -2.921729     206.30
 H       4.364858    -1.763078    -2.199455      24.94
 C       2.513978     0.840033    -2.742373      54.81
 H       2.215143     0.780473    -3.815421      23.79
 C       2.201119     2.200091    -0.678292      57.06
 C       1.712538     3.560053    -0.261073     111.08
 H       2.009146     4.190946    -0.919678      30.54
 O       2.204216     3.880149     1.085934     296.75
 H       3.209545     3.852771     1.066282      27.96
 C       0.168962     3.678184    -0.124727      83.82
 H      -0.037976     3.448439    -1.232132      21.44
 C      -0.212925     5.019722     0.528496     100.58
 O       0.284201     6.289506    -0.098322     231.41
 H       0.523604     6.004401    -1.024219      31.50
 H       0.285465     5.103559     1.536337      24.46
 H      -1.294483     5.268878     0.755798      24.36
 C      -1.419218    -1.012046     0.212343      30.19
 H      -0.800139    -2.097126     0.088856      14.33
 C      -3.335284     0.587064    -0.434539      38.46
 H      -4.499730     0.855439    -0.476704      17.02
 C      -2.469761     1.712632    -0.163829      -1.36
 O      -3.095565     2.982071    -0.014077     160.23
 C      -4.607295     3.199799     0.115750      96.00
 H      -5.079418     2.319499     0.743645      23.63
 H      -4.585810     4.123327     0.526585      26.11
 H      -5.211961     3.299482    -0.918769      23.56
 C      -1.053791     1.561403     0.264335       7.05
 O      -0.227999     2.585900     0.746861     195.77
 C      -0.666765     0.148728     0.320121      27.15
 H       0.446238     0.165832     0.779829      17.39
 C      -2.881687    -0.761358    -0.339723      12.57
 C      -3.893852    -1.869218    -0.634626      48.04
 H      -4.942451    -1.401226    -0.728734      22.31
 O      -3.446626    -2.773186    -1.707156     260.38
 H      -3.930487    -3.550377    -1.702542      19.51
 C      -4.140064    -2.827486     0.747598      73.49
 H      -3.157013    -3.086086     1.409150      19.23
 O      -4.997463    -2.093740     1.533926     357.35
 H      -4.390611    -1.295113     2.044774      21.30
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 C      -5.060550    -4.001252     0.268169      90.72
 O      -4.563755    -4.823983    -0.848231     377.72
 H      -3.870986    -5.422620    -0.499059      27.95
 H      -6.107906    -3.734221     0.091101      28.58
 H      -4.999682    -4.591044     1.305239      25.32
55
name = lig-etoh-frame_572
 C       1.949164     1.965958    -2.145956      89.57
 H       1.136219     2.700708    -2.612895      14.21
 C       3.047407     1.259264    -0.031461      38.56
 H       3.186956     1.428140     1.071065      16.20
 C       3.607040     0.182051    -0.751376      15.56
 O       4.435766    -0.747118    -0.164384     216.54
 C       5.673584    -0.442187     0.786901      97.31
 H       6.533389    -0.305164     0.176267      25.67
 H       5.955566    -1.384996     1.202995      27.16
 H       5.503856     0.452656     1.552747      25.78
 C       3.343445    -0.059960    -2.150993      20.96
 O       3.928590    -1.117726    -2.936653     221.10
 H       4.396278    -1.679904    -2.389436      27.54
 C       2.514812     0.783065    -2.827742      49.18
 H       2.434399     0.556852    -3.946307      25.51
 C       2.208312     2.207280    -0.697551      90.34
 C       1.721019     3.555290    -0.221082      92.04
 H       2.092270     4.332212    -1.254114      25.60
 O       2.227673     3.855818     1.043903     274.38
 H       3.163457     3.861174     1.179196      30.71
 C       0.235712     3.694633    -0.104843      77.98
 H      -0.433668     3.771590    -1.011704      19.20
 C      -0.245172     5.047180     0.524853     103.74
 O       0.247120     6.225305    -0.134561     218.66
 H       0.301938     5.932935    -1.135051      29.94
 H       0.046514     5.289578     1.520013      25.98
 H      -1.344966     4.792552     0.213180      22.42
 C      -1.498553    -1.044079     0.135366      29.94
 H      -0.885632    -1.813977     0.018896      17.95
 C      -3.259448     0.623809    -0.496613      39.84
 H      -4.228969     0.874084    -0.915104      23.35
 C      -2.542323     1.717515    -0.171679      -2.36
 O      -3.094558     2.953032    -0.002036     189.75
 C      -4.576103     3.142327     0.112565      92.10
 H      -4.844180     2.350009     0.731034      27.52
 H      -4.460998     4.317139     0.622918      21.80
 H      -4.882346     3.332217    -0.931921      24.68
 C      -1.044341     1.536266     0.201305      -5.39
 O      -0.267215     2.567963     0.794171     163.49
 C      -0.573931     0.163804     0.356709      17.79
 H       0.344508    -0.038186     0.736115      18.40
 C      -2.892408    -0.777251    -0.312824      21.46
 C      -3.789466    -1.932552    -0.661088      69.64
 H      -4.793939    -1.584124    -0.927164      20.18
 O      -3.482512    -2.780540    -1.779073     245.57
 H      -4.009832    -3.728154    -1.482593      10.26
 C      -4.162532    -2.773153     0.763767     100.31
 H      -3.297626    -2.946001     1.292476      24.49
 O      -5.067414    -2.125011     1.590080     461.97
 H      -4.626620    -1.507018     2.024953      32.17
 C      -5.059423    -4.093916     0.314129      86.47
 O      -4.577349    -4.776974    -0.829734     360.14
 H      -3.975101    -5.450788    -0.460939      26.96
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 H      -6.013452    -3.606244    -0.013565      28.51
 H      -5.285201    -4.667925     1.264956      26.47
55
name = lig-etoh-frame_573
 C       1.907538     1.949913    -2.156727      56.22
 H       1.421109     2.669390    -2.690528      21.07
 C       3.085874     1.332093     0.002805      52.43
 H       3.405871     1.329998     1.051380      16.89
 C       3.523805     0.204903    -0.762701      -2.18
 O       4.486019    -0.749110    -0.148747     244.78
 C       5.646851    -0.496809     0.788226      81.53
 H       6.482284    -0.166677     0.070008      26.05
 H       5.477161    -1.620959     1.093417      23.59
 H       5.542083     0.232156     1.502270      30.48
 C       3.365578    -0.065280    -2.184399       8.58
 O       3.906435    -1.087702    -2.942075     142.46
 H       4.662510    -1.729816    -2.323546      20.00
 C       2.468346     0.801867    -2.912034      47.95
 H       2.542527     0.405108    -4.029575      22.85
 C       2.226004     2.176400    -0.813296      36.07
 C       1.767150     3.557869    -0.236770     119.90
 H       2.029281     4.242394    -0.871316      24.72
 O       2.252015     3.849928     1.039904     262.98
 H       3.307229     3.919039     0.998963      25.98
 C       0.262610     3.709326    -0.067628      64.82
 H      -0.447076     3.724065    -0.867449      18.85
 C      -0.318175     5.061046     0.509391     111.69
 O       0.215143     6.158109    -0.204060     275.80
 H       0.056834     6.050725    -1.138538      31.41
 H      -0.368036     5.202760     1.649575      24.57
 H      -1.258543     4.754049     0.156664      23.74
 C      -1.573867    -0.952526     0.039457      30.62
 H      -1.039952    -2.074115     0.016537      17.37
 C      -3.223791     0.590578    -0.558475      48.62
 H      -4.071060     0.722600    -1.432421      21.90
 C      -2.515026     1.729954    -0.130967      -5.77
 O      -3.074060     2.943892     0.003691     203.52
 C      -4.465519     3.146236     0.112437     112.90
 H      -4.992671     2.305233     0.784426      25.83
 H      -4.682022     3.952283     0.642720      27.21
 H      -4.881969     3.188705    -0.958598      25.06
 C      -1.078726     1.479152     0.161756       1.00
 O      -0.314896     2.553765     0.823067     138.31
 C      -0.572701     0.181450     0.373528      26.44
 H       0.507218    -0.218293     0.698830      19.66
 C      -2.828094    -0.789317    -0.299042      29.62
 C      -3.744351    -2.002305    -0.653973      69.06
 H      -4.706184    -1.526752    -1.006580      18.24
 O      -3.498885    -2.791242    -1.842244     303.62
 H      -3.749578    -3.645089    -1.574649      17.71
 C      -4.199759    -2.754288     0.711169      79.54
 H      -3.144810    -3.020756     1.228008      17.21
 O      -5.161211    -2.146641     1.640809     321.02
 H      -4.652703    -1.428291     2.353849      21.39
 C      -5.058731    -4.106785     0.390506      87.84
 O      -4.593031    -4.772628    -0.802617     310.30
 H      -3.891141    -5.529580    -0.496112      23.99
 H      -5.887597    -3.538244    -0.045583      26.82
 H      -5.617273    -4.936829     1.087732      24.88
55
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name = lig-etoh-frame_574
 C       1.902726     1.874812    -2.208383      42.29
 H       1.539893     2.799185    -2.876519      21.33
 C       3.101411     1.370378    -0.045666      58.91
 H       3.501006     1.453435     0.963351      16.10
 C       3.527561     0.197851    -0.747777      11.74
 O       4.498177    -0.736588    -0.155213     249.46
 C       5.585850    -0.583600     0.733395     101.74
 H       6.461229    -0.225728     0.190176      27.25
 H       5.568681    -1.526931     1.195057      28.44
 H       5.418493     0.148209     1.683037      27.07
 C       3.345777    -0.036992    -2.199957      11.72
 O       3.911904    -1.080533    -2.923228     198.04
 H       4.587524    -1.401397    -2.377243      25.36
 C       2.448352     0.817395    -2.946474      43.25
 H       2.319208     0.634019    -3.986459      22.82
 C       2.254956     2.170985    -0.887344      44.62
 C       1.782819     3.516459    -0.249102     107.29
 H       2.158967     4.622198    -0.901959      17.98
 O       2.321240     3.848752     1.071654     255.14
 H       3.230244     4.048774     0.807620      28.91
 C       0.236320     3.688804    -0.002504      52.90
 H      -0.085335     3.372282    -1.130333      17.15
 C      -0.401312     5.032901     0.493427     105.57
 O       0.192606     6.119619    -0.262154     237.13
 H      -0.188347     6.042849    -1.226654      26.86
 H      -0.540703     5.155233     1.550214      25.42
 H      -1.587681     5.090322     0.306561      22.29
 C      -1.473315    -0.879488    -0.009007      59.11
 H      -1.475585    -1.908437     0.168218      19.21
 C      -3.233959     0.533473    -0.653547      35.77
 H      -3.922449     0.598852    -1.384496      22.35
 C      -2.448818     1.675551    -0.090071      -5.64
 O      -3.018128     2.966923     0.014070     220.52
 C      -4.387084     3.097478     0.102730     119.79
 H      -4.995957     2.331065     0.536467      27.36
 H      -4.874082     4.052310     0.776648      23.42
 H      -5.040611     3.025577    -0.844740      25.44
 C      -1.102485     1.462837     0.194671      12.38
 O      -0.360596     2.541802     0.828676     170.69
 C      -0.634516     0.133649     0.349630      57.19
 H       0.375010    -0.018625     0.542364      22.15
 C      -2.817284    -0.779138    -0.346595       6.45
 C      -3.789889    -2.018795    -0.640299      63.75
 H      -4.638163    -1.329446    -0.878797      19.56
 O      -3.472651    -2.781493    -1.898894     254.01
 H      -3.596705    -3.832151    -1.727826      14.33
 C      -4.208571    -2.802378     0.695433     101.03
 H      -3.322093    -3.049113     1.171005      21.90
 O      -5.221817    -2.135601     1.683828     319.25
 H      -4.715855    -1.661265     2.421586      25.41
 C      -5.090326    -4.073987     0.421580     101.73
 O      -4.586344    -4.820374    -0.771545     345.22
 H      -3.901589    -5.405254    -0.547447      31.18
 H      -5.992421    -3.572072     0.012219      27.09
 H      -5.493320    -4.825192     1.072335      26.63
55
name = lig-etoh-frame_575
 C       1.908679     1.852738    -2.290925      71.55
 H       1.488245     2.633423    -2.789462      23.64
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 C       3.109104     1.357721    -0.161461      46.25
 H       3.430288     1.803540     0.835010      18.01
 C       3.604022     0.180487    -0.740071      17.75
 O       4.457692    -0.729699    -0.202985     255.44
 C       5.514692    -0.624866     0.728382     105.20
 H       6.542839    -0.378112     0.316832      24.74
 H       5.934765    -1.606098     1.291060      24.97
 H       5.250545    -0.011977     1.503968      29.09
 C       3.293487     0.001178    -2.203307      31.48
 O       3.915543    -1.063440    -2.897480     160.45
 H       4.722286    -1.325125    -2.243208      21.04
 C       2.461268     0.801952    -2.928331      45.37
 H       1.974772     0.918501    -4.059067      19.52
 C       2.280760     2.211965    -0.896995      38.52
 C       1.783181     3.553375    -0.241643      95.10
 H       1.989049     4.282555    -0.832689      22.74
 O       2.410663     3.835652     1.099355     269.40
 H       3.336432     4.228217     0.945003      27.33
 C       0.170876     3.600371    -0.008632      72.06
 H       0.102061     3.340439    -1.000988      20.57
 C      -0.517242     4.989070     0.437238     103.02
 O       0.166084     6.099397    -0.306045     256.53
 H      -0.215923     5.902471    -1.201888      29.46
 H      -0.240221     5.217418     1.558020      23.75
 H      -1.524939     5.117235     0.287750      25.74
 C      -1.403702    -0.904977    -0.023590      60.37
 H      -1.236145    -1.963622     0.408456      19.26
 C      -3.219148     0.503013    -0.707791      32.11
 H      -4.285542     0.729984    -1.352695      20.18
 C      -2.441015     1.596673    -0.095611      -4.02
 O      -2.930129     2.985557     0.023895     192.77
 C      -4.417189     3.061009     0.105379     106.11
 H      -4.778976     2.052600     0.600590      25.80
 H      -4.547206     3.942450     0.554636      26.64
 H      -4.918171     3.126738    -0.917081      26.00
 C      -1.108466     1.489708     0.283123      16.68
 O      -0.394997     2.526810     0.827027     219.08
 C      -0.669287     0.131538     0.304583      46.55
 H       0.447149     0.124249     0.531244      19.66
 C      -2.827598    -0.760077    -0.437507      15.13
 C      -3.861262    -1.975549    -0.634174      48.96
 H      -4.782557    -1.411412    -0.820760      20.42
 O      -3.432980    -2.757199    -1.926596     243.80
 H      -3.612024    -3.775690    -1.825884      14.89
 C      -4.252119    -2.866740     0.711732      82.54
 H      -3.299635    -3.133430     1.365600      16.64
 O      -5.241591    -2.127809     1.690723     303.37
 H      -4.683493    -1.774219     2.389808      25.72
 C      -5.130796    -4.019188     0.368429      79.16
 O      -4.586028    -4.877383    -0.744165     321.57
 H      -3.776347    -5.419938    -0.360700      24.60
 H      -6.176742    -3.728007     0.103174      26.85
 H      -5.115611    -4.638435     1.494904      24.56
55
name = lig-etoh-frame_576
 C       1.920152     1.920438    -2.265890      83.72
 H       1.160032     2.598356    -2.885098      20.65
 C       3.123749     1.362025    -0.255068      58.09
 H       3.348243     1.885762     0.629796      22.23
 C       3.674065     0.199318    -0.796235      33.83
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 O       4.418919    -0.775982    -0.266304     236.53
 C       5.489466    -0.666257     0.755003      95.31
 H       6.440000    -0.275217     0.279050      22.24
 H       5.764400    -1.644791     1.083073      24.83
 H       5.081511     0.118950     1.530786      22.95
 C       3.287677    -0.026924    -2.180698      30.21
 O       3.930124    -1.043519    -2.853699     162.27
 H       4.759838    -1.377037    -2.181802      21.21
 C       2.430721     0.802807    -2.955038      34.84
 H       2.120386     0.695818    -3.882699      22.17
 C       2.277503     2.258461    -0.930301      71.47
 C       1.766770     3.558750    -0.147797      76.84
 H       1.879260     4.436904    -1.151169      18.25
 O       2.495874     3.819096     1.110792     286.44
 H       3.407400     4.303464     1.145818      26.89
 C       0.112772     3.510801    -0.029888      60.04
 H      -0.282560     3.357137    -1.190992      16.24
 C      -0.545797     4.953729     0.398100      97.86
 O       0.121637     6.069626    -0.341639     229.48
 H      -0.001348     5.872001    -1.308736      29.22
 H      -0.009167     5.142697     1.306493      24.03
 H      -1.706796     4.902266     0.219705      22.36
 C      -1.453009    -1.050086    -0.026151      31.37
 H      -0.729229    -1.809401     0.406229      17.34
 C      -3.246479     0.552296    -0.750486      44.22
 H      -4.176071     0.794838    -0.931554      21.88
 C      -2.478585     1.584746    -0.138598      -8.29
 O      -2.852725     2.961777     0.021500     186.88
 C      -4.437245     2.985229     0.087031      81.87
 H      -4.560985     2.116415     0.717443      25.00
 H      -4.422799     4.072399     0.638079      22.60
 H      -4.666434     3.230037    -1.007471      23.42
 C      -1.136912     1.483781     0.362971      10.90
 O      -0.407187     2.517764     0.837581     233.30
 C      -0.601228     0.218707     0.277781      14.18
 H       0.457734     0.039765     0.644124      17.99
 C      -2.803088    -0.812312    -0.525049      23.80
 C      -3.907580    -1.917210    -0.634261      48.40
 H      -5.001365    -1.662581    -0.895882      20.33
 O      -3.401519    -2.709299    -1.915964     258.97
 H      -3.737055    -3.565722    -1.806611      18.46
 C      -4.292996    -2.868684     0.739133      82.53
 H      -3.464338    -3.205507     1.326259      18.83
 O      -5.226906    -2.127810     1.654624     307.92
 H      -4.516037    -1.718592     2.453765      19.94
 C      -5.152482    -4.030360     0.341013     104.16
 O      -4.585581    -4.942611    -0.697405     369.75
 H      -3.792610    -5.334749    -0.167966      25.82
 H      -6.208943    -3.888606     0.182889      29.08
 H      -5.002461    -4.413296     1.327257      27.68
55
name = lig-etoh-frame_577
 C       1.895323     2.036102    -2.250097      69.47
 H       1.039076     2.391878    -2.762210      20.91
 C       3.145213     1.400763    -0.315358      47.25
 H       3.484140     1.693397     0.755311      17.85
 C       3.701105     0.259356    -0.900661      17.70
 O       4.407475    -0.866172    -0.315592     260.18
 C       5.447226    -0.651107     0.763704      91.50
 H       6.242840    -0.104570     0.240510      24.30
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 H       5.426140    -1.787350     1.026349      22.66
 H       5.113470     0.001357     1.551631      26.76
 C       3.306087    -0.066669    -2.173430      18.72
 O       3.964954    -1.047634    -2.808307     228.21
 H       4.541894    -1.406151    -2.252377      27.47
 C       2.405521     0.818648    -2.916052      56.21
 H       2.277339     0.243135    -4.058079      21.75
 C       2.261264     2.303920    -0.966460      39.04
 C       1.745565     3.573254    -0.125528     100.09
 H       1.816411     4.319925    -0.708031      24.63
 O       2.535056     3.799191     1.122498     286.44
 H       3.426730     4.193789     0.937795      27.85
 C       0.057478     3.475772    -0.100290      74.20
 H      -0.455690     3.311126    -0.949678      23.07
 C      -0.506402     4.907215     0.330091     100.62
 O       0.056706     6.033942    -0.380431     290.67
 H       0.271065     5.846089    -1.389048      25.85
 H      -0.172319     5.045439     1.408711      24.49
 H      -1.581740     4.714681     0.372388      25.16
 C      -1.471676    -1.101505    -0.014175      18.93
 H      -0.775327    -1.907331     0.121855      15.84
 C      -3.223107     0.598625    -0.733274      39.75
 H      -4.455458     0.794120    -0.709612      18.53
 C      -2.493508     1.636148    -0.181389       9.00
 O      -2.822151     2.902209     0.006896     214.02
 C      -4.359230     2.997519     0.073325     100.48
 H      -4.768620     2.162423     0.745055      25.46
 H      -4.649196     3.827650     0.687997      25.62
 H      -4.725627     3.035424    -0.936942      25.64
 C      -1.180800     1.428105     0.398410       4.33
 O      -0.405887     2.517352     0.873579     224.68
 C      -0.553136     0.223843     0.258050      18.82
 H       0.396443    -0.010271     0.679929      17.54
 C      -2.779480    -0.885070    -0.577350      15.36
 C      -3.932292    -1.897418    -0.651489      72.63
 H      -4.901255    -1.634094    -0.961943      23.54
 O      -3.382438    -2.640993    -1.862470     222.31
 H      -3.984929    -3.572109    -1.817997      16.79
 C      -4.342004    -2.792077     0.715773      81.46
 H      -3.387562    -3.253702     1.231855      19.16
 O      -5.162099    -2.119000     1.618194     411.34
 H      -4.697282    -1.647950     2.222309      30.84
 C      -5.156925    -4.082003     0.313723      83.97
 O      -4.586759    -4.998250    -0.627303     363.73
 H      -3.805623    -5.377040    -0.252684      29.63
 H      -6.263607    -3.896793     0.123102      27.30
 H      -5.205189    -4.765848     1.405202      25.21
55
name = lig-etoh-frame_578
 C       1.858683     2.067289    -2.307345      30.07
 H       0.915221     2.527832    -2.705555      18.67
 C       3.194727     1.453892    -0.317632      45.25
 H       3.519585     1.426721     0.675790      17.73
 C       3.716397     0.303684    -0.959674      15.79
 O       4.391638    -0.921712    -0.353316     242.83
 C       5.364027    -0.647667     0.734279      99.84
 H       6.291734    -0.129305     0.294496      24.08
 H       5.489811    -1.702658     1.125147      24.48
 H       5.015574    -0.100605     1.683404      25.35
 C       3.303704    -0.045056    -2.222498      16.33
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 O       3.987895    -1.073659    -2.812466     157.52
 H       4.567029    -1.652295    -1.968386      17.18
 C       2.407529     0.797079    -2.867594      68.34
 H       2.241530     0.372805    -3.730244      25.94
 C       2.266369     2.365122    -0.941346      53.57
 C       1.708199     3.521381    -0.126227      87.00
 H       1.933338     4.761159    -0.626251      17.63
 O       2.518654     3.768278     1.127162     223.40
 H       3.407930     3.995009     0.668659      27.06
 C       0.048076     3.492414    -0.108884      47.12
 H      -0.444600     3.108129    -1.177941      18.54
 C      -0.427708     4.839149     0.298766     110.11
 O      -0.003224     6.007135    -0.409025     303.05
 H       0.167719     5.710813    -1.320899      29.66
 H      -0.416625     4.986774     1.394511      24.76
 H      -1.575830     4.790552     0.336526      23.40
 C      -1.449456    -1.046832    -0.020716      31.45
 H      -1.177077    -2.212159    -0.210923      14.85
 C      -3.234296     0.576888    -0.670703      38.68
 H      -4.232057     0.602651    -0.760739      19.04
 C      -2.448178     1.646363    -0.205205      14.24
 O      -2.873838     2.881564    -0.002722     250.47
 C      -4.262622     3.012183     0.084159     116.02
 H      -4.911427     2.208238     0.542260      25.69
 H      -4.729851     3.913175     0.651350      24.68
 H      -4.920184     2.822111    -0.896283      23.92
 C      -1.185682     1.378508     0.391490      -2.49
 O      -0.410748     2.505224     0.922007     180.08
 C      -0.586125     0.113468     0.245041      35.30
 H       0.516106     0.012828     0.704019      14.94
 C      -2.769139    -0.874342    -0.564012       2.80
 C      -3.917545    -1.911522    -0.681394      69.11
 H      -4.835401    -1.223342    -1.027889      20.42
 O      -3.402918    -2.613996    -1.781566     286.78
 H      -3.909996    -3.383329    -2.007928      23.40
 C      -4.345490    -2.746073     0.650350      83.94
 H      -3.359075    -3.079739     0.992997      22.55
 O      -5.115940    -2.101561     1.570681     391.64
 H      -4.611369    -1.372744     2.210769      23.58
 C      -5.176961    -4.169431     0.351068      97.00
 O      -4.598637    -5.042105    -0.578255     356.37
 H      -3.650937    -5.498158    -0.351177      24.05
 H      -6.122757    -3.852816    -0.079110      27.69
 H      -5.434875    -4.810452     1.229159      25.93
55
name = lig-etoh-frame_579
 C       1.841637     2.026443    -2.336164      10.43
 H       1.045059     2.714108    -2.754799      18.44
 C       3.256803     1.477699    -0.315088      50.42
 H       3.478378     1.496961     0.808544      14.70
 C       3.724213     0.317119    -0.961850      23.71
 O       4.367030    -0.911956    -0.375557     247.56
 C       5.285553    -0.656246     0.708760     113.70
 H       6.246824    -0.277925     0.439373      26.86
 H       5.734765    -1.622782     1.167416      25.64
 H       4.786905    -0.140536     1.561598      27.14
 C       3.336191    -0.006721    -2.275460      17.11
 O       4.013927    -1.135688    -2.826679     213.78
 H       4.301363    -1.500491    -2.014516      22.52
 C       2.384382     0.823229    -2.813587      56.55
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 H       1.895129     0.560903    -3.971074      21.43
 C       2.290595     2.404723    -0.930876      48.30
 C       1.677883     3.540200    -0.162174     110.97
 H       1.860560     4.368030    -0.582762      21.46
 O       2.457381     3.718023     1.113802     277.69
 H       3.401460     3.841853     0.804471      31.45
 C       0.088462     3.473179    -0.107375      65.32
 H      -0.065745     3.154351    -1.043633      21.34
 C      -0.438331     4.796448     0.312241     109.67
 O      -0.043340     5.986626    -0.408964     290.72
 H      -0.124841     5.684635    -1.435311      26.26
 H      -0.228866     4.977364     1.379578      24.76
 H      -1.511705     4.882693     0.019381      21.75
 C      -1.438589    -1.024749    -0.082459      65.53
 H      -1.374441    -2.018441    -0.212893      19.66
 C      -3.211691     0.480219    -0.584117      54.56
 H      -4.365738     0.602151    -0.964845      16.86
 C      -2.389751     1.590886    -0.202439      15.07
 O      -2.948970     2.905711    -0.006813     230.95
 C      -4.286881     3.013973     0.080713     102.89
 H      -4.664260     2.136338     0.659920      25.03
 H      -4.450296     4.111396     0.406402      23.61
 H      -4.727256     2.975529    -0.880488      25.30
 C      -1.135636     1.352034     0.356447      -2.80
 O      -0.425360     2.469804     0.953337     197.28
 C      -0.622213    -0.025904     0.271843      52.59
 H       0.345430    -0.028732     0.529566      17.97
 C      -2.771529    -0.759633    -0.483027      21.55
 C      -3.919626    -1.871697    -0.710093      72.96
 H      -4.618679    -1.149521    -0.947489      23.35
 O      -3.418944    -2.623121    -1.732135     296.56
 H      -3.935339    -3.364724    -2.100297      23.27
 C      -4.316205    -2.760730     0.550023      71.36
 H      -3.232006    -2.975056     0.955146      19.73
 O      -5.085618    -2.050173     1.551313     358.41
 H      -4.483696    -1.272976     1.969784      24.13
 C      -5.182504    -4.210151     0.376251      77.65
 O      -4.590702    -5.104778    -0.568038     348.56
 H      -3.724654    -5.431901    -0.286408      27.59
 H      -6.009074    -3.813541    -0.291441      26.09
 H      -5.710251    -4.678292     1.421915      24.26
55
name = lig-etoh-frame_580
 C       1.863736     2.005364    -2.252438      18.60
 H       1.296289     2.634132    -2.914138      20.86
 C       3.295284     1.496302    -0.292195      43.25
 H       3.396538     1.771678     0.735907      14.43
 C       3.728620     0.299099    -0.945822      27.97
 O       4.339878    -0.857932    -0.390935     268.52
 C       5.219151    -0.688339     0.709222      92.60
 H       6.193146    -0.046670     0.408343      24.99
 H       5.682885    -1.671335     1.108194      24.87
 H       4.636912    -0.097164     1.409759      28.09
 C       3.405564     0.015577    -2.315975       3.35
 O       3.998135    -1.169978    -2.864031     174.76
 H       4.344563    -1.590528    -1.886771      16.82
 C       2.306266     0.855025    -2.886867      63.07
 H       1.825555     0.776844    -3.771227      23.23
 C       2.333268     2.372411    -0.973230      39.97
 C       1.675877     3.523316    -0.156460      92.52
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 H       1.819741     4.572048    -1.042664      16.23
 O       2.364773     3.660153     1.099991     277.38
 H       3.333516     3.840569     1.090932      30.59
 C       0.192188     3.427485    -0.045617      56.25
 H      -0.032834     3.121378    -1.203768      16.14
 C      -0.515461     4.798383     0.325840     105.44
 O      -0.052191     5.969247    -0.417603     263.74
 H      -0.334590     5.911639    -1.353957      29.88
 H      -0.069540     4.963707     1.346562      24.39
 H      -1.566980     4.671239     0.088439      22.41
 C      -1.483532    -1.048857    -0.169347      55.50
 H      -1.067502    -2.201163    -0.063599      18.22
 C      -3.248647     0.487978    -0.508285      35.02
 H      -4.104425     0.758815    -1.073174      20.23
 C      -2.379725     1.558581    -0.168337     -12.03
 O      -2.936806     2.907385    -0.023664     191.75
 C      -4.377146     3.024565     0.066484      86.89
 H      -4.580294     2.308106     0.940928      24.28
 H      -4.365152     4.099456     0.369476      24.24
 H      -4.711791     3.102452    -1.063566      23.09
 C      -1.064735     1.328738     0.311334       6.93
 O      -0.432251     2.414165     0.946690     185.58
 C      -0.636085    -0.066500     0.324766      33.79
 H       0.562983    -0.298524     0.455696      18.52
 C      -2.793479    -0.733376    -0.372459      38.09
 C      -3.908080    -1.805571    -0.695428      58.36
 H      -4.904992    -1.207265    -1.020616      20.15
 O      -3.404434    -2.660439    -1.739801     220.04
 H      -4.154463    -3.418607    -2.019551      19.19
 C      -4.267621    -2.799532     0.492752      84.75
 H      -3.310733    -3.022520     0.990098      20.10
 O      -5.045774    -1.987275     1.519381     372.57
 H      -4.474412    -1.360200     1.832154      27.81
 C      -5.193312    -4.173757     0.355430      91.14
 O      -4.585310    -5.174880    -0.558453     334.34
 H      -3.698143    -5.466316    -0.154993      25.13
 H      -6.034729    -3.842676    -0.230877      27.82
 H      -5.610529    -4.428503     1.372375      26.60
55
name = lig-etoh-frame_581
 C       1.902917     1.994437    -2.162280      52.01
 H       1.386355     2.637394    -2.954760      20.20
 C       3.291537     1.513362    -0.294752      51.09
 H       3.496711     1.886263     0.729160      16.13
 C       3.721420     0.287608    -0.940593      23.04
 O       4.313602    -0.803295    -0.413256     251.48
 C       5.195027    -0.681908     0.716352     101.36
 H       5.867743     0.056647     0.407311      27.52
 H       5.384054    -1.714073     1.008616      25.44
 H       4.593793    -0.094291     1.538269      26.43
 C       3.432027     0.043339    -2.366420      -2.04
 O       3.955104    -1.178987    -2.880878     170.96
 H       4.524016    -1.665348    -2.116658      20.37
 C       2.298818     0.847814    -2.944707      59.52
 H       1.780891     0.673807    -4.055847      20.43
 C       2.393133     2.313098    -0.981713      29.75
 C       1.751569     3.529722    -0.203255     112.07
 H       1.715777     4.289318    -0.808353      23.81
 O       2.254307     3.614036     1.105367     285.63
 H       3.213063     3.994727     1.166184      27.77
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 C       0.255451     3.382538    -0.019147      72.80
 H      -0.199684     3.149501    -0.912641      21.88
 C      -0.560744     4.800051     0.327184      96.37
 O      -0.060959     5.964255    -0.397819     276.56
 H      -0.360460     5.949878    -1.337502      28.62
 H      -0.279156     5.021368     1.344525      25.39
 H      -1.660631     4.416502     0.493204      21.17
 C      -1.482356    -1.137932    -0.203001      40.96
 H      -0.975018    -1.982131    -0.029196      21.28
 C      -3.279587     0.620369    -0.445373      30.52
 H      -4.191538     0.879066    -1.076751      19.37
 C      -2.404373     1.575480    -0.103965      -7.78
 O      -2.870270     2.875828    -0.053602     174.62
 C      -4.434130     3.057337     0.039372     101.81
 H      -4.925102     2.554689     0.860879      27.53
 H      -4.541823     4.157845     0.505511      24.11
 H      -4.977821     2.914574    -0.848561      26.68
 C      -1.009005     1.291897     0.278733      10.47
 O      -0.406285     2.357703     0.912136     201.85
 C      -0.583016    -0.049322     0.357045      34.83
 H       0.322369    -0.457341     0.474404      21.68
 C      -2.874883    -0.843863    -0.295536      18.96
 C      -3.920797    -1.774465    -0.678521      85.37
 H      -4.847110    -1.497381    -0.989474      22.81
 O      -3.394521    -2.709631    -1.780998     243.01
 H      -4.087835    -3.294057    -1.784213      23.79
 C      -4.248415    -2.812403     0.494996      70.42
 H      -3.297902    -3.227565     0.999074      17.94
 O      -5.013420    -1.952966     1.457019     273.36
 H      -4.259195    -1.251240     1.981336      18.12
 C      -5.174332    -4.079002     0.261959      74.44
 O      -4.593455    -5.233574    -0.522826     322.62
 H      -3.670556    -5.578688    -0.121763      23.16
 H      -6.217126    -3.863487    -0.131655      27.05
 H      -5.309223    -4.334864     1.483961      24.78
55
name = lig-etoh-frame_582
 C       1.922896     1.949574    -2.226488      44.57
 H       1.285855     2.742165    -2.582241      20.51
 C       3.303271     1.479324    -0.292080      54.54
 H       3.733654     1.732426     0.696473      19.26
 C       3.689428     0.319232    -0.976938      32.00
 O       4.292778    -0.772927    -0.429117     222.26
 C       5.124309    -0.630216     0.747028      90.98
 H       6.036263     0.092639     0.461294      24.94
 H       5.325770    -1.806537     0.938710      23.40
 H       4.665184    -0.304992     1.657263      27.45
 C       3.399937     0.065284    -2.397703      11.26
 O       3.904666    -1.168624    -2.909088     201.89
 H       4.535283    -1.538141    -2.358414      25.32
 C       2.357198     0.810420    -2.982857      67.08
 H       2.020578     0.525748    -3.988509      23.22
 C       2.443220     2.307964    -0.917680      26.54
 C       1.820063     3.457013    -0.231380      96.29
 H       1.838004     4.693902    -0.819653      16.16
 O       2.174315     3.597077     1.142852     284.95
 H       2.981081     4.114390     1.077415      27.74
 C       0.224758     3.366424     0.000187      55.87
 H      -0.325461     3.098953    -0.992721      17.92
 C      -0.559353     4.763593     0.374617      96.06
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 O      -0.095267     5.959975    -0.352736     274.76
 H      -0.218934     5.769687    -1.389085      25.50
 H      -0.426538     5.134243     1.452542      23.19
 H      -1.571031     4.529457     0.474820      23.55
 C      -1.482643    -1.145870    -0.159880      27.18
 H      -0.991723    -2.267563    -0.092443      18.11
 C      -3.304477     0.645685    -0.399266      25.56
 H      -4.361311     0.883068    -0.811190      21.36
 C      -2.410181     1.607350    -0.024944      -3.99
 O      -2.839388     2.863514    -0.081219     155.63
 C      -4.454223     3.125766     0.051135      91.05
 H      -5.136367     2.500314     0.773974      25.83
 H      -4.614216     4.124876     0.311374      25.76
 H      -5.179898     2.748906    -0.812040      24.03
 C      -0.992903     1.259566     0.273223      15.69
 O      -0.330530     2.316228     0.877560     203.77
 C      -0.591219    -0.053409     0.316818      35.05
 H       0.487557    -0.439345     0.670908      19.02
 C      -2.941767    -0.876535    -0.273935       3.78
 C      -3.918035    -1.876027    -0.666010      67.55
 H      -4.954950    -1.422544    -1.020429      20.56
 O      -3.380944    -2.731031    -1.816855     209.11
 H      -4.058000    -3.502173    -1.753297      19.00
 C      -4.242365    -2.788469     0.520996      83.12
 H      -3.333675    -3.353842     0.875533      18.16
 O      -4.955071    -1.916417     1.400885     373.00
 H      -4.404354    -1.509116     2.038022      28.81
 C      -5.128924    -3.999298     0.192306      98.90
 O      -4.622351    -5.263397    -0.472685     366.43
 H      -3.764417    -5.549426    -0.195917      31.06
 H      -6.170499    -3.893800    -0.055777      27.63
 H      -5.163571    -4.356583     1.269895      25.78
55
name = lig-etoh-frame_583
 C       1.948573     1.924450    -2.299144      50.68
 H       1.096998     2.652679    -2.398488      18.96
 C       3.355587     1.407493    -0.260688      54.12
 H       3.868293     1.506205     0.670966      21.01
 C       3.659911     0.343465    -1.055347      30.41
 O       4.281736    -0.752376    -0.427529     232.03
 C       5.083007    -0.600903     0.764758     122.25
 H       6.030205    -0.171403     0.682863      27.57
 H       5.505217    -1.563255     0.885765      26.09
 H       4.558184    -0.388320     1.797338      25.05
 C       3.366286     0.045232    -2.373133      12.05
 O       3.825603    -1.129222    -2.965670     132.24
 H       4.769633    -1.393759    -2.321900      19.34
 C       2.438801     0.798555    -2.997759      50.90
 H       2.103445     0.459310    -4.027473      21.92
 C       2.447616     2.313881    -0.915795      73.86
 C       1.800350     3.456529    -0.235464     118.75
 H       2.069602     4.351523    -0.628288      22.00
 O       2.133520     3.599167     1.189594     285.49
 H       2.941841     4.183358     1.183323      28.75
 C       0.130562     3.371876    -0.039071      60.69
 H      -0.180081     3.171331    -1.071801      18.72
 C      -0.505839     4.733034     0.469990      97.26
 O      -0.143944     5.938253    -0.316411     308.54
 H       0.013225     5.643369    -1.223825      30.67
 H      -0.332651     5.044345     1.471787      23.64
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 H      -1.659291     4.700213     0.084341      19.47
 C      -1.509885    -1.137434    -0.064484      53.16
 H      -1.344266    -2.148492    -0.240950      17.63
 C      -3.330612     0.530098    -0.341645      55.89
 H      -4.351273     0.801982    -0.464438      25.63
 C      -2.402804     1.586100     0.034288      -6.14
 O      -2.871820     2.909404    -0.094344     155.79
 C      -4.486878     3.136989     0.058268      88.94
 H      -4.763868     2.506180     0.867728      28.79
 H      -4.538024     4.384851     0.014394      22.94
 H      -4.854790     2.879879    -0.904494      27.14
 C      -1.033660     1.266589     0.291068       5.94
 O      -0.214012     2.282014     0.856342     213.93
 C      -0.599097    -0.124271     0.247273      43.00
 H       0.355912    -0.084925     0.726309      18.26
 C      -2.918959    -0.799980    -0.297658      10.33
 C      -3.930887    -2.017275    -0.699131      69.88
 H      -4.732355    -1.384703    -0.948919      22.58
 O      -3.391821    -2.742535    -1.832353     266.29
 H      -3.724675    -3.771145    -1.929596      17.07
 C      -4.233090    -2.767234     0.510308      89.98
 H      -3.268008    -3.208023     0.896369      19.32
 O      -4.914069    -1.898643     1.357165     364.06
 H      -4.356606    -1.620926     2.219093      23.34
 C      -5.081004    -3.983922     0.178976      88.29
 O      -4.681660    -5.256095    -0.445775     303.15
 H      -3.643530    -5.474540    -0.207718      25.06
 H      -6.111426    -3.772550    -0.206030      25.61
 H      -5.297771    -4.487867     1.293346      23.66
55
name = lig-etoh-frame_584
 C       1.977249     1.949960    -2.288088      73.48
 H       1.012894     2.303270    -2.727148      21.74
 C       3.372481     1.387772    -0.264708      58.07
 H       3.857742     1.403497     0.760749      17.86
 C       3.684138     0.309936    -1.077587      22.29
 O       4.292004    -0.743310    -0.418930     259.16
 C       5.043717    -0.608770     0.803289      94.60
 H       6.059394     0.081390     0.789023      24.17
 H       5.625604    -1.682595     0.896125      21.45
 H       4.444957    -0.358626     1.610460      26.09
 C       3.341126    -0.011467    -2.353188      30.25
 O       3.785085    -1.092248    -3.007429     255.25
 H       4.539940    -1.288486    -2.535890      27.88
 C       2.477506     0.843960    -3.030617      66.43
 H       2.032294     0.470803    -4.089553      21.57
 C       2.441677     2.263118    -0.960686      72.10
 C       1.707812     3.454086    -0.162859     111.14
 H       2.346935     4.441621    -0.802176      17.75
 O       2.124003     3.610652     1.235844     244.99
 H       2.999370     4.097109     1.379378      27.95
 C       0.083502     3.403707    -0.102530      76.81
 H      -0.250879     3.236403    -1.129319      21.65
 C      -0.494966     4.713776     0.503113     109.09
 O      -0.166044     5.915704    -0.266873     307.11
 H       0.174008     5.630571    -1.206450      28.75
 H      -0.244611     4.788981     1.617107      24.03
 H      -1.449928     4.664985     0.196007      24.74
 C      -1.586186    -1.111673     0.021820      51.20
 H      -1.410030    -2.224131    -0.255321      15.94
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 C      -3.329937     0.429051    -0.257870      62.26
 H      -4.499988     0.679181    -0.155221      16.76
 C      -2.437015     1.550778     0.053643       6.61
 O      -2.927706     2.960628    -0.090651     202.46
 C      -4.438061     3.175883     0.027238     102.11
 H      -4.523906     2.670257     1.066896      23.96
 H      -4.475420     4.157803     0.045929      27.85
 H      -4.692668     2.861540    -1.040302      23.93
 C      -1.101479     1.276912     0.322686      -0.48
 O      -0.094881     2.238477     0.823805     168.95
 C      -0.618075    -0.130607     0.198489      39.23
 H       0.422029    -0.108005     0.634603      16.95
 C      -2.855350    -0.773964    -0.355674      14.08
 C      -3.889053    -2.068028    -0.762437      58.43
 H      -4.835227    -1.476191    -1.058475      21.89
 O      -3.397524    -2.773159    -1.856933     337.78
 H      -3.460629    -3.650856    -1.910755      25.27
 C      -4.191256    -2.801204     0.490959      84.08
 H      -3.198240    -2.951262     1.049234      20.70
 O      -4.888704    -1.869565     1.341544     317.01
 H      -4.345185    -1.772984     2.295918      24.07
 C      -5.100602    -4.042120     0.242686      85.32
 O      -4.711629    -5.226860    -0.446780     369.26
 H      -3.804303    -5.454340    -0.260620      30.91
 H      -5.884625    -3.571186    -0.403862      26.72
 H      -5.517279    -4.330910     1.303437      24.91
55
name = lig-etoh-frame_585
 C       1.987519     1.968578    -2.277519      88.85
 H       1.165077     2.233316    -2.922265      22.76
 C       3.345067     1.408276    -0.321402      44.22
 H       3.598836     1.543991     0.695162      17.57
 C       3.747611     0.251834    -1.009227      33.40
 O       4.336803    -0.771563    -0.410544     255.50
 C       5.075817    -0.637104     0.825742     108.66
 H       5.603249     0.278644     0.770709      28.14
 H       5.386797    -1.574666     0.989509      25.15
 H       4.234520    -0.327920     1.626371      24.61
 C       3.284542    -0.027348    -2.383246      33.29
 O       3.756767    -1.086951    -3.068510     200.11
 H       4.620148    -1.499329    -2.582615      25.06
 C       2.491814     0.903619    -3.053094      62.99
 H       2.018371     0.649574    -3.929404      23.30
 C       2.399862     2.219382    -0.965219      40.93
 C       1.672610     3.483086    -0.117221     104.15
 H       1.995727     4.274510    -0.690061      23.87
 O       2.122030     3.621393     1.280932     264.11
 H       3.053094     3.886079     1.284242      28.12
 C       0.123557     3.443408    -0.146364      68.91
 H      -0.454924     3.243650    -1.141812      20.99
 C      -0.485879     4.685853     0.508331      97.38
 O      -0.153108     5.901842    -0.209277     295.38
 H       0.127930     5.722507    -1.131357      28.84
 H      -0.199106     4.608356     1.548923      25.35
 H      -1.727495     4.475223     0.645200      21.45
 C      -1.606497    -1.132535     0.062096      33.63
 H      -1.174026    -2.160067    -0.020488      16.40
 C      -3.375281     0.466746    -0.147246      58.93
 H      -4.374899     0.463258    -0.102447      16.95
 C      -2.527865     1.554006     0.046628       6.16
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 O      -2.955916     2.974567    -0.073553     218.88
 C      -4.308791     3.171458    -0.014407     118.39
 H      -4.800712     2.864358     0.912208      26.56
 H      -4.524333     4.413369     0.197202      23.33
 H      -4.956524     2.676249    -0.808470      24.90
 C      -1.119211     1.271045     0.363744       5.03
 O      -0.021539     2.182878     0.756930     112.89
 C      -0.644318    -0.054461     0.206357      38.70
 H       0.435030    -0.466939     0.314426      15.48
 C      -2.847306    -0.883102    -0.436083      15.94
 C      -3.841127    -2.010931    -0.816389      75.29
 H      -4.849736    -1.762618    -1.162128      21.39
 O      -3.378038    -2.790972    -1.911455     273.59
 H      -3.393105    -3.847900    -1.689626      17.17
 C      -4.117002    -2.854515     0.511597      85.17
 H      -3.196692    -3.007044     1.056247      24.88
 O      -4.875023    -1.847451     1.340140     361.93
 H      -4.452489    -1.736614     2.094055      29.23
 C      -5.144518    -4.085679     0.321632      77.63
 O      -4.736407    -5.192848    -0.465408     327.23
 H      -3.816573    -5.589797    -0.207548      26.07
 H      -5.734464    -3.534103    -0.413647      27.47
 H      -5.898712    -4.077409     1.269967      25.95
55
name = lig-etoh-frame_586
 C       1.978854     1.980167    -2.294957      72.17
 H       1.231388     2.726196    -2.803092      21.70
 C       3.296370     1.420189    -0.390550      48.33
 H       3.376468     1.748355     0.696932      13.70
 C       3.769914     0.215435    -0.970237      38.71
 O       4.413529    -0.851354    -0.408253     249.03
 C       5.026780    -0.616559     0.859873      92.86
 H       5.532538     0.447410     0.788106      26.23
 H       5.529076    -1.684477     1.226679      22.42
 H       4.279472    -0.502420     1.582116      28.63
 C       3.267289    -0.012741    -2.383328      34.35
 O       3.752079    -1.112872    -3.141945     171.52
 H       4.491587    -1.754976    -2.599841      24.50
 C       2.518244     0.947312    -3.020387      52.52
 H       1.900711     0.788266    -4.115791      18.82
 C       2.308018     2.238858    -0.936571      36.16
 C       1.672671     3.464657    -0.100562      87.35
 H       1.744738     4.627937    -0.751474      17.48
 O       2.125650     3.631654     1.300190     250.48
 H       3.115348     3.692558     1.093172      25.76
 C       0.169995     3.441497    -0.155812      80.66
 H      -0.300532     3.264498    -1.032512      21.98
 C      -0.530648     4.634056     0.518601     108.17
 O      -0.136796     5.892995    -0.132692     276.78
 H      -0.072047     5.734447    -1.115120      29.33
 H       0.041657     4.739944     1.516203      24.26
 H      -1.447190     4.499340     0.883421      26.51
 C      -1.549709    -1.157433     0.056519      18.32
 H      -0.982173    -2.110583     0.193558      15.53
 C      -3.403489     0.478619    -0.071387      52.91
 H      -4.611106     0.448007    -0.170494      14.50
 C      -2.592926     1.593529     0.050029       7.88
 O      -2.936260     2.935609    -0.046316     252.20
 C      -4.273854     3.220625    -0.020454     146.44
 H      -4.971446     2.846152     0.842443      25.86
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 H      -4.431638     4.180906    -0.051313      29.25
 H      -5.031519     2.698654    -0.662151      25.64
 C      -1.089546     1.283114     0.392245       8.33
 O      -0.012403     2.129879     0.663916     117.40
 C      -0.691855    -0.019088     0.242593      46.22
 H       0.261610    -0.417444     0.097647      16.48
 C      -2.902407    -0.959134    -0.478815      11.10
 C      -3.809270    -1.977813    -0.832592      73.21
 H      -4.820022    -1.703177    -1.136592      21.61
 O      -3.337904    -2.843125    -1.982344     265.32
 H      -3.417776    -3.716622    -1.440674      16.98
 C      -4.073777    -2.882211     0.556765      69.21
 H      -3.068727    -3.300374     1.033959      20.95
 O      -4.876461    -1.853065     1.301263     277.04
 H      -4.326282    -1.467433     2.267793      19.62
 C      -5.191070    -4.045621     0.367115      81.92
 O      -4.745331    -5.176469    -0.480709     293.04
 H      -3.976887    -5.734328    -0.046561      27.10
 H      -5.884702    -3.569972    -0.379097      27.93
 H      -5.952389    -4.183666     1.244360      26.16
55
name = lig-etoh-frame_587
 C       1.927563     2.072569    -2.294111      50.32
 H       1.478944     2.957934    -2.605653      18.15
 C       3.235253     1.419802    -0.393277      60.77
 H       3.441345     1.652732     0.634304      13.57
 C       3.732344     0.193888    -1.002547      31.98
 O       4.495896    -0.939023    -0.417065     240.81
 C       4.984406    -0.601481     0.913960     131.19
 H       5.654002     0.207962     0.939582      29.76
 H       5.733759    -1.246612     1.178830      26.57
 H       4.125757    -0.590647     1.725387      24.81
 C       3.327415    -0.029836    -2.347644      25.12
 O       3.749203    -1.145362    -3.201183     253.54
 H       4.181044    -1.660908    -2.658542      32.83
 C       2.496279     0.973511    -3.027673      19.74
 H       2.209925     0.847832    -3.932708      21.82
 C       2.217045     2.290994    -0.930202      62.59
 C       1.680322     3.492680    -0.138891     110.59
 H       1.857935     4.461908    -0.569716      21.44
 O       2.151522     3.637374     1.266916     269.31
 H       3.156269     3.629958     1.176193      27.52
 C       0.186250     3.387353    -0.105998      71.39
 H      -0.074876     3.249003    -1.291466      18.85
 C      -0.478332     4.605128     0.582792      93.09
 O      -0.133205     5.881003    -0.070509     230.22
 H      -0.401596     5.790172    -1.067522      27.87
 H       0.187986     4.858667     1.383208      24.36
 H      -1.678152     4.546811     0.847458      22.08
 C      -1.527667    -1.162806     0.000087      42.96
 H      -0.965299    -2.145237     0.230015      15.94
 C      -3.460707     0.415992    -0.066363      73.41
 H      -4.437909     0.679705    -0.236235      15.57
 C      -2.567778     1.601041     0.085568       4.49
 O      -2.894904     2.879184    -0.009809     205.14
 C      -4.353337     3.242098    -0.000770      92.40
 H      -4.671076     2.916684     1.003522      25.66
 H      -4.350495     4.468105    -0.376097      22.83
 H      -4.784385     2.749809    -0.992764      23.47
 C      -1.104792     1.318863     0.379345      13.30
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 O      -0.038661     2.101151     0.570332     165.37
 C      -0.759726    -0.044986     0.285269      30.78
 H       0.455269    -0.063260     0.099690      15.37
 C      -2.884841    -0.916001    -0.417316      13.55
 C      -3.814259    -2.038910    -0.838883      54.14
 H      -4.780281    -1.455452    -1.049608      22.20
 O      -3.307099    -2.895031    -2.010515     288.91
 H      -3.385165    -3.719574    -1.619672      23.02
 C      -4.084411    -2.895289     0.598245      83.89
 H      -3.207238    -3.360796     0.953246      23.59
 O      -4.845818    -1.870740     1.300386     363.63
 H      -4.417505    -1.288610     1.898594      28.55
 C      -5.230971    -3.964276     0.350559      93.79
 O      -4.754824    -5.165298    -0.475483     308.86
 H      -4.159916    -5.670947     0.018097      31.67
 H      -6.057181    -3.588353    -0.229854      28.74
 H      -5.640189    -4.548872     1.338638      24.29
55
name = lig-etoh-frame_588
 C       1.896448     2.169456    -2.280916      48.72
 H       1.511976     3.107951    -2.894472      19.15
 C       3.160965     1.392400    -0.362295      55.72
 H       3.642741     1.444633     0.650589      15.56
 C       3.680885     0.164010    -1.040600      28.72
 O       4.558991    -0.973509    -0.425873     235.79
 C       4.946338    -0.595904     0.976802     108.76
 H       5.605514     0.392184     1.041726      26.89
 H       5.922482    -1.295381     1.154428      25.01
 H       4.169594    -0.598677     1.696296      26.83
 C       3.375459    -0.038699    -2.370515       9.80
 O       3.727473    -1.131754    -3.241160     144.51
 H       4.148362    -1.873197    -2.460162      20.70
 C       2.481100     1.000707    -2.965411      64.43
 H       2.405917     0.792500    -4.204710      21.54
 C       2.202276     2.306734    -0.923243      33.10
 C       1.696952     3.508561    -0.150208      95.62
 H       2.213741     4.565911    -0.693777      18.77
 O       2.196579     3.631720     1.210486     294.67
 H       3.138654     3.717078     1.336865      29.08
 C       0.167148     3.324561    -0.092265     102.12
 H       0.043129     3.366734    -1.099789      22.68
 C      -0.416870     4.608965     0.663180     104.14
 O      -0.148456     5.866535    -0.044729     283.38
 H      -0.581344     5.895457    -0.885015      30.90
 H       0.112421     4.702321     1.658230      24.98
 H      -1.451506     4.533079     0.652759      24.45
 C      -1.524440    -1.158496    -0.064592      56.97
 H      -1.178585    -2.153657    -0.049885      18.26
 C      -3.439902     0.374856    -0.105602      73.39
 H      -4.494676     0.781564    -0.374820      13.39
 C      -2.497016     1.517260     0.145088      20.48
 O      -2.878298     2.863749     0.027711     209.27
 C      -4.395617     3.286813    -0.038535     114.09
 H      -4.632082     3.127201     1.030141      27.02
 H      -4.297526     4.251170    -0.270830      28.50
 H      -4.660076     2.794292    -0.936642      27.03
 C      -1.204320     1.306412     0.326103      20.48
 O      -0.061998     2.108139     0.494560     203.63
 C      -0.746479    -0.049683     0.316329      33.99
 H       0.245181     0.054929     0.418165      20.71
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 C      -2.856377    -0.851391    -0.307369      11.62
 C      -3.815264    -2.121415    -0.819578      52.73
 H      -4.680762    -1.582538    -1.086743      24.12
 O      -3.295090    -2.911620    -1.996849     260.48
 H      -3.394419    -4.012574    -1.915261      18.07
 C      -4.178020    -2.873562     0.568584      74.86
 H      -3.189567    -3.346401     1.070432      19.41
 O      -4.824339    -1.903471     1.304575     305.76
 H      -4.244170    -1.173308     1.781993      24.04
 C      -5.233304    -3.953122     0.333486      91.40
 O      -4.784817    -5.123026    -0.478023     296.41
 H      -4.095070    -5.628561     0.136931      26.65
 H      -6.225217    -3.520211    -0.025514      27.73
 H      -5.354698    -4.486296     1.350850      25.18
55
name = lig-etoh-frame_589
 C       1.913325     2.222991    -2.319266      42.80
 H       1.487965     2.835510    -3.024063      20.39
 C       3.105506     1.303799    -0.328031      42.99
 H       3.624165     1.426679     0.635744      18.01
 C       3.644202     0.126888    -1.038599      18.37
 O       4.584955    -0.933935    -0.421570     212.76
 C       5.001172    -0.591595     0.999095     109.67
 H       5.161354     0.461216     1.031009      26.92
 H       5.606462    -1.410847     1.222603      26.55
 H       4.109900    -0.674082     1.764007      26.75
 C       3.359782    -0.011931    -2.451635      14.45
 O       3.715991    -1.109872    -3.224466     203.81
 H       4.064363    -1.875849    -2.684323      23.31
 C       2.483083     1.022294    -2.921006      61.00
 H       2.362027     0.911988    -3.935762      25.02
 C       2.256826     2.298229    -0.899529      23.35
 C       1.777883     3.538313    -0.150213     103.57
 H       2.076327     4.369298    -0.776374      23.47
 O       2.234496     3.617294     1.169051     297.95
 H       3.226972     3.884723     1.240440      25.60
 C       0.173406     3.364538    -0.080884      72.89
 H      -0.269675     3.488843    -1.203074      20.14
 C      -0.342730     4.613480     0.718659     102.09
 O      -0.150912     5.858067    -0.006677     267.67
 H      -0.709612     5.858841    -0.826146      28.57
 H      -0.184036     4.519922     1.816585      24.59
 H      -1.511069     4.408450     0.722408      21.59
 C      -1.500670    -1.119706    -0.102788      39.51
 H      -1.313685    -2.251779    -0.453985      17.88
 C      -3.384826     0.418581    -0.156178      59.78
 H      -4.430830     0.524996    -0.476181      24.13
 C      -2.551182     1.453998     0.182029      16.37
 O      -2.883685     2.864689     0.067109     188.83
 C      -4.338271     3.292525    -0.060079      97.89
 H      -5.022210     3.260152     0.905656      25.51
 H      -4.256823     4.519568    -0.216713      22.86
 H      -5.002665     2.610802    -0.859873      23.76
 C      -1.211953     1.231791     0.276296      21.46
 O      -0.101834     2.104810     0.451419     164.49
 C      -0.724876    -0.052806     0.333298      42.29
 H       0.410538    -0.191208     0.835367      18.92
 C      -2.886346    -0.875913    -0.242404      27.28
 C      -3.782574    -2.187497    -0.771624      53.41
 H      -4.780124    -1.823523    -1.281221      19.33
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 O      -3.283577    -2.924398    -1.956608     301.52
 H      -3.544233    -3.859572    -2.041634      22.58
 C      -4.242068    -2.854720     0.480407     106.90
 H      -3.424966    -3.201689     1.035861      20.90
 O      -4.830293    -1.917781     1.342412     310.61
 H      -3.984811    -1.273931     1.657146      19.81
 C      -5.232601    -3.994959     0.336764      87.85
 O      -4.818285    -5.067815    -0.481818     370.78
 H      -4.028635    -5.482397    -0.021645      29.34
 H      -6.191557    -3.580421     0.153080      28.74
 H      -5.269418    -4.218536     1.536591      25.28
55
name = lig-etoh-frame_590
 C       2.004942     2.178598    -2.321519      38.79
 H       1.283108     2.788290    -3.009367      19.77
 C       3.077801     1.181880    -0.310796      53.77
 H       3.359145     1.516535     0.693406      20.30
 C       3.628551     0.082905    -1.022463      17.49
 O       4.569297    -0.839915    -0.416410     225.57
 C       4.987882    -0.594824     0.995906      91.53
 H       5.142455     0.545342     1.086279      24.31
 H       5.681348    -1.457626     1.353402      24.93
 H       4.123820    -0.804393     1.626293      28.18
 C       3.318469     0.026399    -2.460881      23.40
 O       3.701943    -1.073845    -3.222451     203.65
 H       4.072834    -1.780482    -2.720626      24.84
 C       2.491549     1.048251    -2.903027      60.91
 H       2.150930     1.001778    -4.082423      22.43
 C       2.330573     2.289796    -0.911816      54.52
 C       1.837059     3.507720    -0.161305      88.82
 H       1.819288     4.501960    -0.972846      21.06
 O       2.294852     3.615430     1.155704     296.33
 H       3.182700     4.033724     0.991728      25.67
 C       0.196681     3.479860    -0.109422      67.58
 H      -0.435284     3.558627    -0.943706      21.91
 C      -0.360818     4.584238     0.755038     110.19
 O      -0.138222     5.855302     0.052734     249.26
 H      -0.733727     5.704905    -0.758730      28.49
 H      -0.126867     4.639820     1.824135      25.41
 H      -1.425304     4.347145     0.823752      23.67
 C      -1.511168    -1.123011    -0.141862      40.29
 H      -1.130939    -1.988445    -0.514842      21.39
 C      -3.378306     0.426624    -0.216760      69.23
 H      -4.425770     0.432825    -0.479958      26.62
 C      -2.649316     1.488618     0.186027       6.60
 O      -2.927172     2.856685     0.112228     242.29
 C      -4.291769     3.299680    -0.072378     143.07
 H      -5.026844     3.222749     0.738956      28.02
 H      -4.263739     4.326591    -0.363351      27.48
 H      -4.952881     2.803726    -0.674688      29.59
 C      -1.127619     1.178355     0.251734      -1.52
 O      -0.152061     2.093390     0.441480     116.45
 C      -0.638511    -0.118094     0.364428      60.06
 H       0.175175    -0.405951     0.834028      22.96
 C      -2.916876    -0.966350    -0.249789      33.93
 C      -3.792435    -2.176254    -0.771572      90.33
 H      -4.684971    -1.867376    -1.207844      22.47
 O      -3.247564    -2.924127    -1.902573     290.09
 H      -3.755157    -3.752090    -1.914395      22.10
 C      -4.278882    -2.867318     0.401337      97.07
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 H      -3.329146    -3.313595     0.996293      18.88
 O      -4.839313    -1.905636     1.387818     403.42
 H      -4.157617    -1.456469     1.679067      28.51
 C      -5.230611    -4.021235     0.404190      89.43
 O      -4.848736    -5.024403    -0.495517     377.12
 H      -3.978156    -5.386242    -0.286367      31.80
 H      -6.286888    -3.712203     0.091582      26.68
 H      -5.376931    -4.260392     1.532789      26.11
55
name = lig-etoh-frame_591
 C       2.096057     2.140205    -2.275420      39.57
 H       1.281232     2.760968    -2.604431      20.98
 C       3.046708     1.121515    -0.297812      75.10
 H       3.087437     1.356793     0.810281      21.43
 C       3.627433     0.056842    -0.997380      25.51
 O       4.540323    -0.740756    -0.422923     243.46
 C       4.933512    -0.596751     0.976496     109.36
 H       5.426779     0.338970     1.227889      26.00
 H       5.878373    -1.133390     1.205143      24.71
 H       4.028731    -0.823558     1.595069      25.36
 C       3.292463     0.033121    -2.387799      30.48
 O       3.678244    -1.019573    -3.246049     151.55
 H       4.259822    -1.704588    -2.494610      19.50
 C       2.498508     1.041469    -3.002403      57.93
 H       2.019793     0.925385    -3.998347      22.52
 C       2.406376     2.257921    -0.961061      77.63
 C       1.804415     3.472429    -0.228161      97.27
 H       1.920090     4.440311    -0.763171      24.00
 O       2.375101     3.637289     1.137606     300.86
 H       3.235438     4.109424     1.029714      27.33
 C       0.227822     3.548048    -0.103322      55.96
 H      -0.368739     3.622983    -1.096732      20.08
 C      -0.404974     4.566505     0.812914     102.53
 O      -0.135956     5.845472     0.116695     247.47
 H      -0.570073     5.753516    -0.725081      31.60
 H       0.237581     4.817192     1.720991      23.56
 H      -1.515139     4.367129     0.866555      22.18
 C      -1.548794    -1.147731    -0.160560      43.17
 H      -0.808552    -2.073194    -0.408173      17.64
 C      -3.433171     0.357953    -0.275863      45.52
 H      -4.589590     0.570823    -0.421386      23.59
 C      -2.636057     1.527419     0.158550     -10.95
 O      -2.983918     2.844969     0.160354     217.90
 C      -4.265982     3.303402    -0.069366      97.13
 H      -4.767593     3.206708     1.019025      23.40
 H      -4.203126     4.384424    -0.550127      24.08
 H      -4.818510     2.721844    -1.079469      22.98
 C      -1.086267     1.172448     0.251585     -10.32
 O      -0.173911     2.114340     0.461330     105.51
 C      -0.619810    -0.201248     0.361720      33.40
 H       0.472048    -0.551902     0.798119      18.23
 C      -2.908978    -1.030664    -0.316964      41.37
 C      -3.821650    -2.092040    -0.817972      72.32
 H      -4.786609    -1.504445    -1.180455      21.21
 O      -3.193050    -2.935141    -1.832876     213.34
 H      -4.014758    -3.683061    -1.804532      16.51
 C      -4.265933    -2.915840     0.450459      94.05
 H      -3.366948    -3.384763     0.741516      21.61
 O      -4.873253    -1.915905     1.402162     317.02
 H      -4.105204    -1.329603     1.997885      20.54
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 C      -5.274295    -4.017664     0.470919      94.55
 O      -4.874031    -5.011834    -0.527235     309.10
 H      -3.859594    -5.335656    -0.496165      25.82
 H      -6.212290    -3.804512     0.010723      25.65
 H      -5.474362    -4.583126     1.523386      24.32
55
name = lig-etoh-frame_592
 C       2.154078     2.115685    -2.256453      61.30
 H       1.377798     2.872050    -2.486296      22.37
 C       2.996907     1.143375    -0.259159      62.82
 H       3.015328     1.004265     0.795346      21.05
 C       3.598794     0.099839    -0.970813      27.81
 O       4.541107    -0.683777    -0.430214     257.27
 C       4.895368    -0.580506     0.948503     115.27
 H       5.396318     0.384229     1.275079      26.18
 H       5.818693    -1.215636     0.930118      24.63
 H       4.077887    -0.813619     1.715029      26.08
 C       3.266025     0.020912    -2.350632      38.30
 O       3.679954    -0.983100    -3.227550     263.24
 H       4.274273    -1.452767    -2.750959      30.04
 C       2.509856     1.004053    -3.096464      44.13
 H       2.049466     0.750248    -4.099870      20.16
 C       2.475347     2.206119    -0.947324      22.71
 C       1.754920     3.441795    -0.261252      88.93
 H       2.309306     4.464749    -0.685250      19.46
 O       2.442528     3.660772     1.111556     257.45
 H       3.382690     4.085077     1.118544      25.73
 C       0.223862     3.528610    -0.097001      69.58
 H       0.000505     3.665303    -1.182729      20.40
 C      -0.406115     4.593080     0.862751     101.53
 O      -0.144663     5.846234     0.175225     258.38
 H      -0.367218     5.892579    -0.801817      30.28
 H       0.308144     4.676001     1.638301      24.47
 H      -1.521058     4.409064     1.110710      22.22
 C      -1.504635    -1.231260    -0.152284      53.37
 H      -1.089896    -2.188193    -0.159264      19.05
 C      -3.485017     0.322035    -0.296157      32.15
 H      -4.475228     0.549423    -0.360744      21.82
 C      -2.559132     1.450504     0.086090     -16.66
 O      -2.991052     2.831062     0.206165     218.26
 C      -4.293968     3.298294    -0.098432     118.06
 H      -4.712699     3.313494     0.863464      26.14
 H      -4.121648     4.363283    -0.454011      25.31
 H      -4.575192     2.757734    -0.904677      28.56
 C      -1.109091     1.177117     0.267315      -4.55
 O      -0.154568     2.170013     0.505121     142.64
 C      -0.642917    -0.241257     0.345101      39.02
 H       0.404659    -0.378671     0.399336      20.27
 C      -2.899795    -1.007558    -0.418417      24.27
 C      -3.887323    -1.998790    -0.861925      82.70
 H      -4.653331    -1.390700    -1.225528      23.81
 O      -3.182948    -2.959930    -1.748824     275.81
 H      -3.806075    -3.589122    -1.944104      25.09
 C      -4.256849    -2.917442     0.555995      63.23
 H      -3.192147    -3.437755     0.724500      17.74
 O      -4.879661    -1.931801     1.414808     350.38
 H      -4.416174    -1.439948     2.168430      25.74
 C      -5.327099    -4.057913     0.495650      89.47
 O      -4.879801    -5.021794    -0.582737     357.67
 H      -3.969363    -5.249599    -0.426703      30.03
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 H      -6.281699    -3.632350     0.082263      27.31
 H      -5.453052    -4.632409     1.457892      25.82
55
name = lig-etoh-frame_593
 C       2.178556     2.085991    -2.325657      70.86
 H       1.636096     2.994704    -2.755769      23.36
 C       2.971422     1.153924    -0.187657      53.13
 H       2.991243     0.886371     0.911170      17.92
 C       3.544730     0.182890    -0.976096      28.20
 O       4.549646    -0.660752    -0.443596     249.53
 C       4.909874    -0.556483     0.935614     110.86
 H       5.111663     0.501239     1.147449      26.13
 H       5.541255    -1.515267     0.870685      23.32
 H       4.199866    -0.869020     1.716444      27.66
 C       3.234051     0.015884    -2.380890      34.79
 O       3.690384    -0.955870    -3.206058     201.25
 H       4.536353    -1.541360    -2.859648      23.54
 C       2.514554     0.980291    -3.104309      55.09
 H       2.238057     0.620483    -4.228795      19.48
 C       2.471826     2.203757    -0.876568      41.73
 C       1.822728     3.454941    -0.226527      97.95
 H       2.180327     4.232777    -0.866971      24.84
 O       2.483519     3.672015     1.103036     282.57
 H       3.412073     3.937383     0.950953      27.37
 C       0.208730     3.458004    -0.091418      70.84
 H      -0.026784     3.619303    -1.168695      20.80
 C      -0.364401     4.624755     0.857180      98.22
 O      -0.159716     5.880714     0.231628     279.72
 H      -0.172383     5.825902    -0.787751      29.34
 H       0.239503     4.478733     1.845198      23.23
 H      -1.350375     4.439697     1.261046      23.86
 C      -1.482616    -1.317420    -0.117842      35.56
 H      -1.380880    -2.492817    -0.027432      16.19
 C      -3.427601     0.325073    -0.283196      28.52
 H      -4.623841     0.477323    -0.373750      14.60
 C      -2.499196     1.349908    -0.001317       6.14
 O      -2.933881     2.785552     0.255779     171.98
 C      -4.284116     3.305823    -0.117022      97.45
 H      -5.189514     3.396698     0.755993      23.52
 H      -4.122750     4.319982    -0.417862      24.89
 H      -4.824084     2.527093    -0.989602      23.07
 C      -1.156889     1.173966     0.279551       9.93
 O      -0.126683     2.219235     0.560103     155.07
 C      -0.703963    -0.197724     0.281735      41.37
 H       0.448171    -0.257290     0.149187      17.74
 C      -2.883902    -0.919542    -0.515693      19.91
 C      -3.920177    -1.989186    -0.858284      53.41
 H      -4.811394    -1.508048    -1.469226      20.42
 O      -3.180125    -2.962953    -1.674678     243.86
 H      -3.744745    -3.720555    -2.115357      21.68
 C      -4.250895    -2.885159     0.642307      64.71
 H      -3.307696    -3.218409     0.941341      22.87
 O      -4.896935    -1.958190     1.438528     371.00
 H      -4.487685    -1.553944     2.233287      27.22
 C      -5.349777    -4.096585     0.446425      70.72
 O      -4.901281    -5.025669    -0.633169     335.22
 H      -3.994882    -5.290727    -0.260430      27.71
 H      -6.257781    -3.493161     0.320090      28.33
 H      -5.434618    -4.631891     1.555244      26.24
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name = lig-etoh-frame_594
 C       2.194374     2.104669    -2.381289      79.78
 H       1.944700     2.918650    -3.003458      24.26
 C       2.961862     1.138242    -0.093856      46.86
 H       2.965356     1.144018     0.968318      19.80
 C       3.521635     0.214275    -1.009585      13.04
 O       4.526943    -0.649164    -0.485163     216.37
 C       4.926653    -0.563713     0.917201     101.23
 H       5.184890     0.507559     1.105502      25.03
 H       5.610545    -1.381327     1.102069      24.33
 H       4.067265    -0.852458     1.652713      25.49
 C       3.228919     0.015288    -2.394562      25.16
 O       3.726447    -0.973162    -3.192532     194.53
 H       4.663602    -1.487650    -2.887146      23.19
 C       2.513870     0.955039    -3.084540      52.69
 H       2.397405     0.800860    -4.091576      22.50
 C       2.378655     2.245672    -0.859250      59.56
 C       1.926328     3.464901    -0.154972      86.38
 H       1.831094     4.231793    -1.159437      21.93
 O       2.500816     3.680344     1.089357     270.35
 H       3.459942     3.835431     0.826403      25.96
 C       0.209220     3.399784    -0.069819      57.59
 H      -0.372292     3.441809    -1.077367      21.03
 C      -0.272660     4.615985     0.843811      96.15
 O      -0.169049     5.939439     0.282963     300.70
 H      -0.061754     5.671891    -0.613734      31.49
 H       0.185357     4.547993     1.801846      25.58
 H      -1.430091     4.452308     1.119702      22.68
 C      -1.544889    -1.355831    -0.091637      28.53
 H      -1.410414    -2.441931     0.013748      16.40
 C      -3.366570     0.354490    -0.280677      56.69
 H      -4.352152     0.445882    -0.380164      16.32
 C      -2.500771     1.360104    -0.052252      14.06
 O      -2.885250     2.716155     0.298131     176.61
 C      -4.307205     3.249108    -0.136289     118.75
 H      -5.031945     3.291044     0.536787      29.19
 H      -4.092498     4.346906    -0.633799      24.23
 H      -4.805124     2.752665    -0.817562      29.87
 C      -1.156324     1.166947     0.276033      11.07
 O      -0.126610     2.215888     0.623407     151.27
 C      -0.722102    -0.152491     0.184777      38.11
 H       0.413483    -0.213647     0.178972      19.14
 C      -2.859562    -0.897177    -0.582050       4.60
 C      -3.927306    -2.044222    -0.832624      72.08
 H      -4.810031    -1.886910    -1.426464      20.58
 O      -3.168649    -2.967177    -1.624984     238.20
 H      -3.782440    -3.718367    -2.077028      20.90
 C      -4.284958    -2.834902     0.658906      51.69
 H      -3.261429    -3.068983     1.238935      20.97
 O      -4.947496    -1.971277     1.479804     324.22
 H      -4.321787    -1.613004     2.358952      21.86
 C      -5.309997    -4.100884     0.407628      90.49
 O      -4.932959    -5.017248    -0.659158     332.55
 H      -4.097604    -5.486775    -0.237247      26.78
 H      -6.283168    -3.592826     0.316032      28.42
 H      -5.432387    -4.607119     1.386941      26.91
55
name = lig-etoh-frame_595
 C       2.207615     2.154894    -2.355555      59.37
 H       2.100004     3.023612    -3.114937      19.65
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 C       2.921950     1.172058    -0.096332      59.14
 H       3.057222     1.399016     1.002972      18.20
 C       3.536915     0.192032    -0.985499       8.74
 O       4.501940    -0.660289    -0.535562     229.95
 C       4.907153    -0.566231     0.893477     105.37
 H       5.433929     0.384400     1.162079      25.89
 H       5.899661    -1.097373     1.237842      23.94
 H       4.039039    -0.595330     1.489728      27.42
 C       3.257502    -0.003140    -2.374519      25.28
 O       3.790739    -1.024154    -3.188637     231.50
 H       4.495813    -1.299174    -2.755327      29.64
 C       2.506312     0.950525    -3.033358      43.07
 H       2.493096     1.091415    -4.299111      21.15
 C       2.286276     2.242742    -0.897010      39.31
 C       1.916212     3.478444    -0.179148     106.55
 H       1.868403     4.335679    -0.814507      24.73
 O       2.521136     3.701532     1.068088     297.48
 H       3.534311     3.856968     1.023004      27.46
 C       0.215905     3.371062    -0.024006      62.77
 H      -0.375190     3.320360    -0.892558      23.31
 C      -0.232276     4.584269     0.841765      99.17
 O      -0.163413     5.990816     0.322796     271.04
 H       0.024225     5.797464    -0.662469      29.27
 H       0.333734     4.692667     1.817710      23.98
 H      -1.266502     4.429260     0.821047      24.36
 C      -1.638247    -1.283801    -0.091494      41.50
 H      -1.197546    -2.324029    -0.024249      17.50
 C      -3.307684     0.366122    -0.320673      57.85
 H      -4.477934     0.589011    -0.424488      17.20
 C      -2.505041     1.489298    -0.039608      18.96
 O      -2.889940     2.655467     0.318170     201.75
 C      -4.253156     3.214117    -0.175092      78.75
 H      -4.874831     3.242211     0.976373      21.33
 H      -4.075056     4.076634    -0.634627      26.90
 H      -4.791987     2.560003    -1.162085      23.06
 C      -1.106242     1.174267     0.246239       5.31
 O      -0.158713     2.152599     0.704290     186.15
 C      -0.700007    -0.166959     0.090523      43.09
 H       0.361357    -0.291733     0.338357      19.86
 C      -2.861297    -0.973941    -0.594101      18.92
 C      -3.889307    -2.137640    -0.764542      88.91
 H      -4.908278    -1.956919    -1.227931      22.58
 O      -3.143902    -2.999708    -1.607384     301.64
 H      -3.766447    -3.604863    -1.807064      25.59
 C      -4.294772    -2.802130     0.630753      85.23
 H      -3.426680    -3.092223     1.107315      26.83
 O      -5.019433    -1.953442     1.562597     416.07
 H      -4.416795    -1.608759     2.117975      31.06
 C      -5.235288    -4.056269     0.379553      99.64
 O      -4.960252    -5.013578    -0.669100     337.69
 H      -4.289312    -5.608529    -0.445072      33.15
 H      -6.268411    -3.770390     0.038207      26.98
 H      -5.393624    -4.758220     1.393287      24.55
55
name = lig-etoh-frame_596
 C       2.215899     2.205019    -2.304337      49.42
 H       2.028070     3.105554    -2.781121      21.58
 C       2.870823     1.234089    -0.196799      63.19
 H       3.222013     1.476984     0.793056      19.61
 C       3.541980     0.170426    -0.913594       8.01
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 O       4.514105    -0.702802    -0.553825     234.77
 C       4.935067    -0.529667     0.859456     106.42
 H       5.413799     0.471119     1.008666      26.55
 H       5.707087    -1.202789     1.065773      26.08
 H       3.974763    -0.412811     1.550909      24.12
 C       3.277641    -0.025406    -2.366592      -4.87
 O       3.846734    -1.067222    -3.177844     140.55
 H       4.658242    -1.388538    -2.389606      18.58
 C       2.512150     1.002109    -3.020146      58.73
 H       2.545231     1.082682    -3.971593      25.68
 C       2.237014     2.212541    -0.957955      39.94
 C       1.816350     3.482388    -0.236255      89.29
 H       2.153904     4.636983    -0.573014      19.76
 O       2.534171     3.717197     1.073365     299.97
 H       3.466163     4.004041     1.110271      28.46
 C       0.265190     3.355195     0.062303      58.96
 H      -0.208079     3.329417    -1.041887      21.14
 C      -0.209583     4.575118     0.846341      89.13
 O      -0.135836     6.017296     0.329942     240.04
 H       0.014763     6.195003    -0.649911      29.74
 H       0.304964     4.668950     1.800723      24.51
 H      -1.391999     4.329793     0.884239      21.53
 C      -1.638995    -1.184931    -0.107237      38.43
 H      -1.001153    -2.145233    -0.141902      16.77
 C      -3.302814     0.381441    -0.403403      49.93
 H      -4.322017     0.648159    -0.469341      19.20
 C      -2.447375     1.510675    -0.015902      10.28
 O      -2.951094     2.686131     0.329314     238.55
 C      -4.208577     3.114157    -0.180358     116.56
 H      -4.609739     3.242509     0.668888      28.04
 H      -3.947461     4.259111    -0.620550      23.54
 H      -4.527215     2.516035    -0.853801      30.50
 C      -1.054161     1.191300     0.184311      10.40
 O      -0.193224     2.072639     0.800870     173.62
 C      -0.680495    -0.186756     0.024072      37.01
 H       0.333735    -0.538703     0.557127      18.64
 C      -2.946408    -1.031584    -0.549114      22.37
 C      -3.847051    -2.196496    -0.677618      95.98
 H      -4.819958    -1.750435    -1.051702      22.84
 O      -3.113753    -3.053119    -1.602606     232.67
 H      -3.826383    -3.906248    -1.665927      15.45
 C      -4.313402    -2.797107     0.596715      80.09
 H      -3.309357    -3.291801     1.032863      21.91
 O      -5.107793    -1.945955     1.611661     312.52
 H      -4.352868    -1.317726     2.142534      22.57
 C      -5.188833    -4.033903     0.374464     111.84
 O      -4.979088    -5.010228    -0.701562     298.90
 H      -4.255292    -5.735571    -0.547767      29.52
 H      -6.116364    -3.697567    -0.044153      28.96
 H      -5.295232    -4.562485     1.279859      28.49
55
name = lig-etoh-frame_597
 C       2.203894     2.226869    -2.301328      37.86
 H       1.786434     3.248480    -2.639865      17.88
 C       2.880175     1.242551    -0.313426      67.76
 H       3.256840     1.525227     0.669121      18.99
 C       3.507955     0.156133    -0.914121       8.08
 O       4.540832    -0.753378    -0.522704     230.15
 C       4.956641    -0.456301     0.822411     105.71
 H       5.368265     0.569602     0.740208      26.02
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 H       5.443063    -1.549373     0.964545      22.87
 H       4.183434    -0.509504     1.519185      28.38
 C       3.268567    -0.018433    -2.364416       0.19
 O       3.925013    -1.091221    -3.103756     196.96
 H       4.484001    -1.606431    -2.512572      23.96
 C       2.562908     1.056437    -2.966484      64.47
 H       2.540597     0.970346    -4.254339      21.62
 C       2.210828     2.234006    -0.967372      45.39
 C       1.750232     3.518370    -0.239872      95.40
 H       2.008353     4.347340    -0.759852      25.35
 O       2.507165     3.703092     1.107974     249.61
 H       3.426998     4.203826     0.898643      24.75
 C       0.325722     3.357536     0.104480      73.85
 H      -0.003987     3.349836    -0.860239      22.79
 C      -0.258033     4.589242     0.840596     105.05
 O      -0.095577     6.031305     0.334728     270.03
 H      -0.083296     6.225016    -0.589553      31.84
 H       0.205449     4.602067     1.836486      24.95
 H      -1.216042     4.416779     1.161003      25.85
 C      -1.568347    -1.140574    -0.161689      38.94
 H      -1.170726    -2.124685    -0.198193      18.67
 C      -3.301541     0.393172    -0.491838      96.17
 H      -4.406959     0.651695    -0.580263      22.16
 C      -2.377481     1.413807    -0.018510       0.44
 O      -2.977450     2.744986     0.351178     211.53
 C      -4.119021     3.098266    -0.194861      97.61
 H      -5.085455     3.332408     0.764506      22.65
 H      -4.022650     4.008931    -0.593096      26.47
 H      -4.635796     2.174906    -0.933242      21.11
 C      -1.018411     1.198210     0.115172      20.29
 O      -0.197177     2.027515     0.893360     145.69
 C      -0.645288    -0.168039     0.021676      48.55
 H       0.170362    -0.535833     0.460062      21.12
 C      -3.011137    -0.988759    -0.446806      34.73
 C      -3.830194    -2.183938    -0.638383      77.63
 H      -4.678516    -1.686867    -1.148951      21.46
 O      -3.125607    -3.139696    -1.593815     258.10
 H      -3.502187    -4.046283    -1.576379      18.45
 C      -4.282364    -2.846847     0.633104      97.45
 H      -3.426071    -3.228825     1.090379      22.20
 O      -5.147218    -1.958048     1.629454     302.92
 H      -4.623127    -1.109798     1.976379      22.71
 C      -5.187127    -4.014992     0.340057      82.71
 O      -4.971945    -5.019001    -0.752391     293.61
 H      -4.190173    -5.605129    -0.454731      29.76
 H      -6.155390    -3.454185     0.118798      27.63
 H      -5.327620    -4.463452     1.536381      25.43
55
name = lig-etoh-frame_598
 C       2.151509     2.269158    -2.353131      60.61
 H       1.585960     3.036277    -2.900343      16.64
 C       2.951869     1.214015    -0.351975      62.64
 H       3.155584     1.490687     0.709745      17.32
 C       3.482738     0.107485    -1.011157      16.14
 O       4.518696    -0.777086    -0.487671     215.44
 C       4.998798    -0.438549     0.775723     116.46
 H       5.606563     0.480921     0.758393      26.82
 H       5.503654    -1.313221     1.066764      26.07
 H       4.146006    -0.471856     1.617844      25.04
 C       3.272702    -0.011090    -2.343533      19.28
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 O       3.968465    -1.080717    -3.027594     201.86
 H       4.420609    -1.770751    -2.429115      22.44
 C       2.647294     1.076272    -3.014280      56.86
 H       2.469202     0.955840    -3.961227      24.73
 C       2.202543     2.296670    -0.929115      67.87
 C       1.760083     3.499521    -0.152086      79.32
 H       1.690833     4.279786    -1.212163      23.68
 O       2.464673     3.688771     1.118255     275.07
 H       3.259331     4.169414     0.865301      28.06
 C       0.325416     3.384839     0.144244      48.24
 H      -0.248140     3.222655    -0.915064      18.72
 C      -0.298691     4.628255     0.858711      96.01
 O      -0.049283     6.021931     0.354671     221.11
 H      -0.279514     5.916597    -0.654331      29.44
 H       0.290514     4.672588     1.839265      24.77
 H      -1.439301     4.515519     1.232237      22.65
 C      -1.545547    -1.155694    -0.246474      36.42
 H      -1.382388    -2.337114    -0.172261      16.79
 C      -3.324145     0.402806    -0.550271      69.49
 H      -4.415774     0.648916    -0.728088      22.79
 C      -2.388285     1.352871    -0.043918     -16.36
 O      -2.909508     2.743207     0.389721     189.61
 C      -4.187164     3.073908    -0.197299     130.04
 H      -4.977841     3.203670     0.352396      29.11
 H      -4.131957     4.099005    -0.917804      25.15
 H      -4.578692     2.445894    -0.828614      30.84
 C      -0.979975     1.201907     0.088826      14.97
 O      -0.171041     2.031287     0.953305      97.49
 C      -0.612727    -0.128085     0.036205      28.67
 H       0.544507    -0.452094     0.367105      17.26
 C      -2.945417    -0.893674    -0.333152      32.57
 C      -3.839446    -2.149754    -0.653597      59.51
 H      -4.724694    -1.899566    -1.361488      19.02
 O      -3.127423    -3.201627    -1.571815     240.21
 H      -3.433136    -4.087344    -1.438742      18.82
 C      -4.247766    -2.879240     0.700463      90.68
 H      -3.314581    -3.132601     1.377825      18.93
 O      -5.160191    -1.996321     1.598194     354.02
 H      -4.757348    -1.203261     1.846555      26.99
 C      -5.254159    -4.004843     0.347150     110.41
 O      -4.947229    -5.015766    -0.773821     327.47
 H      -4.209597    -5.433514    -0.359132      32.74
 H      -6.173711    -3.486814     0.227453      30.36
 H      -5.432696    -4.451434     1.228617      29.73
55
name = lig-etoh-frame_599
 C       2.093242     2.260643    -2.400245      72.87
 H       1.502525     2.780116    -3.128862      21.96
 C       3.012303     1.223604    -0.332854      45.82
 H       3.130521     1.236644     0.732505      17.41
 C       3.501623     0.065457    -1.044383      12.35
 O       4.451035    -0.785475    -0.479699     263.57
 C       5.029762    -0.436578     0.786600     106.57
 H       5.804908     0.376726     0.876274      26.42
 H       5.885976    -1.180737     1.200243      24.35
 H       4.292891    -0.182707     1.470741      29.01
 C       3.305803    -0.029463    -2.383940      30.24
 O       3.988461    -1.044211    -2.974183     153.39
 H       4.245696    -1.800364    -2.142283      17.47
 C       2.717113     1.099853    -3.044194      70.40
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 H       2.381749     0.950727    -4.248486      19.24
 C       2.250110     2.313445    -0.927068      42.89
 C       1.768430     3.471035    -0.099450     112.70
 H       1.615865     4.211960    -0.784791      25.27
 O       2.405270     3.686677     1.101364     286.85
 H       3.372311     4.078021     1.057708      25.97
 C       0.209986     3.403975     0.154517      59.41
 H      -0.330285     3.174519    -0.660474      22.71
 C      -0.334033     4.679568     0.948252     109.96
 O      -0.010558     5.978767     0.338912     263.88
 H      -0.437083     5.752970    -0.520134      30.01
 H       0.255823     4.759278     1.801623      25.74
 H      -1.359630     4.578127     0.924746      25.18
 C      -1.527705    -1.207174    -0.294930      52.99
 H      -1.323156    -2.185886    -0.202237      19.68
 C      -3.351475     0.439921    -0.565841      67.31
 H      -4.341303     0.652318    -0.821928      21.77
 C      -2.441353     1.401131    -0.072824     -22.83
 O      -2.833792     2.697423     0.405137     154.27
 C      -4.225410     3.116745    -0.252765      74.29
 H      -5.204123     3.222118     0.658625      22.19
 H      -4.117656     3.885743    -0.917412      27.05
 H      -4.581454     2.267380    -1.151101      21.52
 C      -0.963043     1.207341     0.130678      -4.95
 O      -0.138944     2.071680     0.967594     139.45
 C      -0.528171    -0.155127     0.049369      29.22
 H       0.463640    -0.188738     0.090638      19.56
 C      -2.847957    -0.867633    -0.296794      31.52
 C      -3.841201    -2.140457    -0.680299      60.94
 H      -4.721905    -2.023689    -1.240487      20.35
 O      -3.104918    -3.214343    -1.541323     193.28
 H      -3.641922    -4.127699    -1.186172      11.86
 C      -4.235438    -2.867912     0.762799      92.93
 H      -3.372211    -3.077108     1.362893      20.94
 O      -5.165698    -2.074733     1.527435     325.39
 H      -4.596957    -1.134731     1.880576      21.03
 C      -5.316722    -3.998700     0.349140      80.84
 O      -4.924287    -4.985962    -0.759886     254.28
 H      -4.124336    -5.501227    -0.282772      26.38
 H      -6.292198    -3.511529     0.016459      26.43
 H      -5.618656    -4.890637     1.261121      23.77
55
name = lig-etoh-frame_600
 C       2.083129     2.169928    -2.409296      60.51
 H       1.341293     2.760809    -3.109453      22.02
 C       3.045982     1.241838    -0.319321      49.70
 H       3.151967     1.089186     0.783556      17.38
 C       3.525382     0.106749    -0.987953      14.48
 O       4.391856    -0.809600    -0.467262     245.11
 C       5.115158    -0.432333     0.825070      92.27
 H       5.733386     0.490472     0.625245      26.80
 H       5.750940    -1.245751     1.130257      26.00
 H       4.339888     0.000959     1.568616      25.79
 C       3.343483    -0.013030    -2.456841      19.71
 O       4.005942    -1.046768    -2.939308     229.03
 H       4.149891    -1.504631    -2.230240      26.98
 C       2.735206     1.112889    -3.108887      64.18
 H       2.556775     1.014842    -4.141484      22.69
 C       2.327322     2.284859    -0.975185      33.22
 C       1.713801     3.422919    -0.084687      92.97
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 H       1.862151     4.663529    -0.505219      16.45
 O       2.366170     3.699958     1.120675     282.94
 H       3.366715     3.810189     1.162906      27.98
 C       0.103266     3.396566     0.217970      54.31
 H      -0.480137     3.290353    -0.847240      19.19
 C      -0.336879     4.713615     1.020738      93.33
 O       0.016991     5.917243     0.296313     247.23
 H      -0.448752     5.949073    -0.541775      30.32
 H       0.065405     4.751954     2.143475      23.19
 H      -1.498328     4.597989     0.903317      22.17
 C      -1.440487    -1.203520    -0.282064      44.29
 H      -1.034134    -2.342675    -0.301298      18.93
 C      -3.320568     0.464402    -0.528100      64.01
 H      -4.461943     0.599337    -0.893800      23.60
 C      -2.453310     1.508207    -0.078485       0.44
 O      -2.815469     2.658050     0.374588     163.76
 C      -4.278178     3.103562    -0.284331      93.92
 H      -4.778118     3.214508     0.497936      28.18
 H      -3.986298     4.149050    -0.874807      23.68
 H      -4.457542     2.374613    -0.953346      28.52
 C      -0.990405     1.175148     0.223370      -9.85
 O      -0.127417     2.127935     0.939475     164.41
 C      -0.500176    -0.173649     0.028094      36.50
 H       0.718627    -0.213271    -0.095202      17.76
 C      -2.837120    -0.905961    -0.373711      25.95
 C      -3.780390    -2.166151    -0.662700      54.31
 H      -4.852415    -1.820783    -1.098794      20.04
 O      -3.092154    -3.206491    -1.478776     254.09
 H      -3.703698    -3.874939    -1.321075      19.39
 C      -4.289366    -2.853927     0.758847      88.21
 H      -3.319970    -3.234333     1.303251      20.33
 O      -5.147805    -2.111041     1.464764     405.17
 H      -4.676185    -1.482910     1.946808      30.14
 C      -5.374012    -4.065806     0.376546     105.72
 O      -4.878875    -4.948874    -0.718462     332.20
 H      -4.255902    -5.608082    -0.390474      31.10
 H      -6.151383    -3.547429    -0.155260      30.35
 H      -5.680388    -4.669195     1.058106      27.42
55
name = lig-etoh-frame_601
 C       2.088476     2.069101    -2.390508      54.85
 H       1.420106     2.776637    -2.722369      24.73
 C       3.068404     1.249584    -0.295990      59.97
 H       3.118659     1.322547     0.778073      18.95
 C       3.539479     0.195152    -0.978809      10.49
 O       4.349577    -0.850206    -0.418449     227.42
 C       5.171741    -0.386410     0.832561      82.31
 H       5.641695     0.460075     0.316379      25.92
 H       5.597338    -1.443827     1.087545      24.00
 H       4.543603    -0.151592     1.677369      27.25
 C       3.378203     0.079090    -2.448141      12.93
 O       4.022417    -1.068111    -2.971462     135.17
 H       4.387172    -1.625230    -2.007618      14.81
 C       2.743850     1.086693    -3.158294      65.99
 H       2.678527     1.056943    -4.347404      19.65
 C       2.368882     2.267562    -1.030490      26.22
 C       1.651800     3.466717    -0.124005      91.60
 H       1.916112     4.316814    -0.558864      21.90
 O       2.333648     3.685867     1.202913     281.78
 H       3.273538     3.636712     0.991057      29.34
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 C       0.046672     3.379396     0.253493      81.55
 H      -0.377852     3.600240    -0.667914      23.17
 C      -0.380758     4.713670     1.063223     110.66
 O       0.053079     5.862415     0.261992     256.15
 H      -0.426807     6.083899    -0.606177      29.37
 H      -0.224158     4.799083     2.061925      27.14
 H      -1.441599     4.690639     1.207424      25.95
 C      -1.336839    -1.207204    -0.240702      33.22
 H      -0.941679    -2.125662    -0.447054      18.01
 C      -3.274493     0.433910    -0.475441      40.76
 H      -4.228724     0.518666    -0.742524      17.05
 C      -2.384221     1.515696    -0.068560      18.10
 O      -2.866577     2.698883     0.324920     199.92
 C      -4.214037     3.130832    -0.326475      73.90
 H      -4.860784     3.278698     0.846880      21.07
 H      -3.981806     4.169822    -0.575825      24.24
 H      -4.594868     2.264084    -1.039959      22.08
 C      -1.039622     1.133785     0.324844       9.55
 O      -0.151589     2.167889     0.886940     208.09
 C      -0.470481    -0.143056    -0.009597      45.40
 H       0.530560    -0.402060    -0.089117      18.41
 C      -2.836860    -0.966840    -0.506630       2.54
 C      -3.729477    -2.176436    -0.617187      97.59
 H      -4.567333    -1.690168    -1.009704      24.15
 O      -3.081427    -3.156084    -1.410241     250.11
 H      -3.829963    -3.964802    -1.559149      15.80
 C      -4.326198    -2.919978     0.686413      97.92
 H      -3.486082    -3.394476     1.190561      24.67
 O      -5.154777    -2.107592     1.438488     369.52
 H      -4.659763    -1.519666     2.188091      24.88
 C      -5.358547    -4.104137     0.336782      70.53
 O      -4.836398    -4.925601    -0.682972     297.76
 H      -4.300730    -5.669323    -0.379143      29.85
 H      -6.147090    -3.512205    -0.197816      28.54
 H      -5.936860    -4.603341     1.451556      24.42
55
name = lig-etoh-frame_602
 C       2.102419     2.006971    -2.353605      63.31
 H       1.420374     2.935554    -2.666041      21.52
 C       3.065920     1.305064    -0.257562      48.13
 H       3.143962     1.592725     0.805271      20.09
 C       3.585268     0.235805    -1.012554       4.07
 O       4.290509    -0.875689    -0.350244     234.31
 C       5.191948    -0.381939     0.789063      94.18
 H       5.880908     0.366591     0.342569      24.88
 H       5.723240    -1.376191     0.967819      23.92
 H       4.647955    -0.171934     1.747345      24.98
 C       3.455111     0.133091    -2.397385      11.49
 O       4.029906    -1.091548    -2.983781     162.39
 H       4.649567    -1.462697    -2.313417      21.92
 C       2.737824     1.040034    -3.219373      63.27
 H       2.785270     1.088795    -4.368626      20.62
 C       2.361721     2.251428    -1.019967      51.83
 C       1.600372     3.481695    -0.135594      69.29
 H       1.842709     4.377534    -1.084420      18.57
 O       2.295876     3.646106     1.274362     230.37
 H       3.267454     3.643029     0.915572      26.16
 C       0.064455     3.423336     0.271483      72.64
 H      -0.524498     3.666942    -0.737243      19.75
 C      -0.453277     4.697147     1.053243      91.26
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 O       0.095921     5.823929     0.247580     211.48
 H      -0.449705     5.892772    -0.570150      30.32
 H       0.018705     4.927093     2.145639      23.62
 H      -1.595534     4.754804     1.226233      24.23
 C      -1.320244    -1.186193    -0.228563      30.06
 H      -0.823461    -2.196000    -0.553448      18.23
 C      -3.174291     0.334426    -0.417135      29.39
 H      -4.362276     0.594294    -0.592976      17.09
 C      -2.312958     1.426699    -0.041993      13.56
 O      -2.938678     2.776822     0.256468     227.02
 C      -4.140943     3.138622    -0.253942     145.14
 H      -4.830640     3.180003     0.403649      30.39
 H      -4.020228     4.112410    -0.679434      27.78
 H      -4.764451     2.605963    -1.043581      26.22
 C      -1.059285     1.141832     0.399339      21.58
 O      -0.206623     2.159295     0.841233     196.91
 C      -0.481760    -0.098272    -0.027856      35.41
 H       0.635161    -0.387218     0.050705      18.98
 C      -2.737343    -0.996526    -0.587059      25.60
 C      -3.705743    -2.178007    -0.563600      88.26
 H      -4.605784    -1.683202    -1.212077      21.34
 O      -3.072055    -3.120848    -1.369321     269.10
 H      -3.685405    -3.838265    -1.725549      20.82
 C      -4.349918    -3.011531     0.610240      95.65
 H      -3.514568    -3.510124     1.224766      22.98
 O      -5.172112    -2.065418     1.445174     318.06
 H      -4.617067    -1.646507     2.291452      23.54
 C      -5.356639    -4.089627     0.320560     114.12
 O      -4.804461    -4.944470    -0.665627     312.62
 H      -4.211949    -5.683742    -0.211972      28.04
 H      -6.223429    -3.595100    -0.121720      30.13
 H      -5.725176    -4.370966     1.149255      31.04
55
name = lig-etoh-frame_603
 C       2.092909     2.023702    -2.367349      62.18
 H       1.587082     2.720845    -2.935150      23.69
 C       3.068451     1.372987    -0.231194      32.62
 H       3.284686     1.578828     0.828240      17.69
 C       3.655331     0.247569    -0.982895      11.93
 O       4.226196    -0.860798    -0.279281     276.25
 C       5.208068    -0.424376     0.712962     111.74
 H       6.041438     0.297880     0.548456      26.71
 H       5.943300    -1.266142     0.905881      24.86
 H       4.734185    -0.016792     1.643379      25.80
 C       3.557984     0.109462    -2.397404       8.12
 O       4.028838    -1.074548    -3.000167     146.22
 H       4.846168    -1.396969    -2.466935      23.76
 C       2.730370     1.012318    -3.209508      48.85
 H       2.751509     1.021078    -4.302212      23.38
 C       2.300397     2.236762    -0.935618      40.81
 C       1.586064     3.499631    -0.167460      92.20
 H       1.595834     4.254317    -0.797175      25.62
 O       2.262236     3.600977     1.270206     253.09
 H       3.225062     3.867610     1.216267      28.10
 C       0.069263     3.497277     0.221462      65.29
 H      -0.549379     3.387433    -0.643121      23.46
 C      -0.485411     4.703951     1.068377     113.22
 O       0.116300     5.791174     0.241111     225.73
 H      -0.383926     5.687124    -0.566686      31.43
 H       0.186190     4.835593     1.823650      26.10
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 H      -1.573840     4.739979     1.029095      25.30
 C      -1.319922    -1.190542    -0.278179      55.41
 H      -0.833734    -2.152352    -0.418333      20.71
 C      -3.118086     0.254477    -0.373001      51.91
 H      -4.078339     0.535192    -0.371577      21.12
 C      -2.351431     1.349290    -0.004267      -3.44
 O      -2.931786     2.792205     0.192989     211.00
 C      -4.124505     3.180383    -0.226648     113.89
 H      -5.206023     3.163278     0.542427      22.84
 H      -4.082222     4.149669    -0.973274      23.66
 H      -4.634998     2.640745    -1.168409      23.87
 C      -1.014824     1.189549     0.420522      19.78
 O      -0.252845     2.133433     0.830850     180.53
 C      -0.485111    -0.075730    -0.004046      30.97
 H       0.617033    -0.068344     0.273562      19.90
 C      -2.609530    -1.011554    -0.569179      48.24
 C      -3.744688    -2.164065    -0.573554      96.65
 H      -4.557335    -1.894842    -1.132239      25.09
 O      -3.019669    -3.110835    -1.380421     297.89
 H      -3.633018    -3.736558    -1.666418      24.16
 C      -4.350017    -3.021665     0.608447      94.30
 H      -3.545141    -3.490119     1.209285      23.01
 O      -5.173002    -2.030687     1.462809     357.06
 H      -4.630805    -1.734450     2.091049      31.15
 C      -5.352068    -4.018465     0.238823      84.11
 O      -4.778134    -5.019681    -0.654150     304.96
 H      -4.127251    -5.479101    -0.128211      30.37
 H      -6.283575    -3.640084    -0.183930      27.86
 H      -5.622589    -4.626496     1.432755      24.14
55
name = lig-etoh-frame_604
 C       2.102115     2.043186    -2.406606      49.54
 H       1.552028     2.687754    -3.198556      20.26
 C       3.114591     1.385455    -0.221923      38.42
 H       3.382994     1.429542     0.819766      17.70
 C       3.711023     0.271939    -0.924347       7.61
 O       4.184228    -0.814747    -0.215346     287.51
 C       5.252683    -0.473887     0.660285     103.45
 H       5.916722     0.401883     0.360861      27.13
 H       5.940859    -1.381522     0.980041      24.43
 H       4.787203    -0.033337     1.529087      26.93
 C       3.631932     0.068915    -2.413815       4.59
 O       4.031500    -1.044417    -3.016946     104.49
 H       5.029483    -1.423762    -2.607700      22.55
 C       2.747753     0.999437    -3.085850      43.41
 H       2.578345     0.882640    -4.307846      21.90
 C       2.178178     2.263603    -0.882198      52.75
 C       1.596236     3.458225    -0.136572      93.09
 H       1.643515     4.692669    -0.631762      19.81
 O       2.227568     3.568650     1.223158     265.77
 H       3.052967     4.091642     1.366202      29.99
 C       0.039420     3.496482     0.160483      62.05
 H      -0.536384     3.317812    -0.806079      22.44
 C      -0.442843     4.702690     1.017836     107.16
 O       0.108260     5.778354     0.228213     201.07
 H      -0.208634     5.655829    -0.749413      29.40
 H       0.152704     4.674964     2.033144      24.75
 H      -1.556894     4.699124     1.069400      25.40
 C      -1.220848    -1.205707    -0.333990      55.45
 H      -0.818828    -2.229354    -0.264179      23.69
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 C      -3.088579     0.234810    -0.326517      54.66
 H      -4.287518     0.359611    -0.298673      22.12
 C      -2.421316     1.337358     0.052745       5.89
 O      -2.851034     2.750916     0.153356     183.35
 C      -4.258401     3.240782    -0.287208     122.55
 H      -4.853591     3.253167     0.471526      30.35
 H      -4.094671     4.153745    -0.749165      28.24
 H      -4.276918     2.410363    -1.043359      25.10
 C      -1.012915     1.202518     0.348212      13.63
 O      -0.240960     2.155851     0.881035     169.49
 C      -0.474347    -0.047269     0.073943      39.65
 H       0.567449    -0.023096     0.328335      20.65
 C      -2.608264    -1.052017    -0.492080      23.42
 C      -3.734669    -2.167243    -0.614143      69.62
 H      -4.763355    -1.797335    -1.163932      21.74
 O      -2.941110    -3.116919    -1.424242     204.53
 H      -3.718668    -3.928470    -1.593688      14.85
 C      -4.337219    -2.918256     0.655197      87.01
 H      -3.505103    -3.439979     1.193011      22.52
 O      -5.169317    -2.026961     1.452974     312.73
 H      -4.404904    -1.536474     2.164580      21.85
 C      -5.362009    -4.025025     0.210659     108.43
 O      -4.764213    -5.103470    -0.646316     305.32
 H      -3.932446    -5.347763    -0.135038      28.18
 H      -6.259259    -3.608667    -0.302172      28.11
 H      -5.538996    -4.511849     0.990597      29.85
55
name = lig-etoh-frame_605
 C       2.102696     2.079321    -2.405805      40.94
 H       1.447006     2.680149    -3.022967      21.24
 C       3.148542     1.381041    -0.251502      40.71
 H       3.329430     1.382499     0.858402      18.00
 C       3.735197     0.303080    -0.920756       6.72
 O       4.163999    -0.777463    -0.167157     276.97
 C       5.320838    -0.499828     0.648607      94.93
 H       5.746498     0.292933     0.002153      26.43
 H       5.764545    -1.451384     0.906093      25.86
 H       4.883156    -0.133906     1.656739      25.65
 C       3.650517     0.084575    -2.349735      14.49
 O       4.074931    -1.045880    -3.050385     220.98
 H       4.774274    -1.396766    -2.702991      29.38
 C       2.782602     0.970237    -2.964824      57.98
 H       2.515264     0.798732    -3.927394      24.83
 C       2.096917     2.282674    -0.906913      30.70
 C       1.606819     3.494182    -0.081222     114.24
 H       1.902162     4.336950    -0.461850      28.04
 O       2.186120     3.531867     1.178443     245.35
 H       2.906450     4.279857     1.136973      27.57
 C       0.004076     3.411814     0.106611      78.62
 H      -0.428578     3.515342    -0.929008      23.56
 C      -0.364330     4.669507     0.934743     114.65
 O       0.085586     5.803840     0.205495     264.89
 H       0.026710     5.693728    -0.755596      31.94
 H      -0.170874     4.639371     2.005149      26.08
 H      -1.473029     4.691656     1.188079      25.90
 C      -1.111560    -1.219524    -0.364425      32.10
 H      -0.709434    -2.287919    -0.147714      21.83
 C      -3.177601     0.234523    -0.278914      65.35
 H      -4.230635     0.115587    -0.357690      23.40
 C      -2.450428     1.418426     0.119313      14.81
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 O      -2.767912     2.700378     0.130029     129.96
 C      -4.310944     3.221612    -0.387935      63.20
 H      -4.897466     3.274822     0.764926      22.75
 H      -4.052520     4.392075    -0.584074      22.75
 H      -4.498635     2.372802    -1.013228      24.55
 C      -1.057276     1.203888     0.242903      15.42
 O      -0.208139     2.214092     0.951442     173.28
 C      -0.453376    -0.048261     0.157851      27.08
 H       0.721964    -0.220074     0.316712      20.04
 C      -2.653684    -1.101116    -0.390638     -10.13
 C      -3.690555    -2.168595    -0.679324      87.14
 H      -4.476025    -1.696034    -1.131686      24.49
 O      -2.909068    -3.155771    -1.481714     267.73
 H      -3.372374    -3.940728    -1.504571      22.05
 C      -4.328792    -2.802999     0.675598      85.05
 H      -3.473288    -3.319145     1.219525      22.20
 O      -5.119692    -2.020745     1.463877     383.32
 H      -4.665684    -1.345810     1.982256      29.62
 C      -5.332633    -4.029892     0.145677      67.98
 O      -4.745362    -5.174078    -0.637652     280.14
 H      -3.766813    -5.314024    -0.305322      24.87
 H      -6.134014    -3.575482    -0.423238      26.32
 H      -5.878087    -4.646885     1.257076      23.20
55
name = lig-etoh-frame_606
 C       2.087509     2.113798    -2.313606      48.53
 H       1.330261     2.695731    -2.880124      20.90
 C       3.114051     1.408934    -0.300932      47.84
 H       3.163100     1.458462     0.760386      19.27
 C       3.744451     0.312659    -0.928074      20.68
 O       4.144135    -0.763802    -0.129646     264.77
 C       5.355090    -0.499695     0.661494      96.13
 H       6.023244     0.073709    -0.045921      25.87
 H       5.821326    -1.626692     0.668309      23.54
 H       5.211913    -0.127554     1.638147      27.76
 C       3.649955     0.103393    -2.248074      15.53
 O       4.096017    -1.031477    -3.093351     118.19
 H       4.868651    -1.617086    -2.464519      21.60
 C       2.800351     0.976305    -2.865664      45.90
 H       2.429498     0.607179    -4.024929      21.41
 C       2.131645     2.259076    -0.964565      44.62
 C       1.571706     3.478834    -0.055447     102.13
 H       2.165518     4.392315    -0.835307      22.81
 O       2.173392     3.508681     1.171638     282.56
 H       2.820448     4.167088     1.006248      30.14
 C       0.025096     3.350730     0.087765     101.74
 H      -0.437373     3.467134    -0.904461      23.83
 C      -0.348044     4.617855     0.842607     108.09
 O       0.071324     5.863251     0.191801     261.11
 H       0.150114     5.657741    -0.756532      32.94
 H       0.033973     4.693786     1.897190      26.02
 H      -1.445932     4.699928     0.931304      26.18
 C      -1.097577    -1.227859    -0.333403      41.76
 H      -0.578276    -2.130569    -0.240474      22.79
 C      -3.270667     0.214549    -0.219799      47.29
 H      -4.416267     0.221788    -0.405001      21.99
 C      -2.458952     1.438068     0.143217       1.97
 O      -2.746850     2.709389     0.103200     116.73
 C      -4.296083     3.185212    -0.383548      94.95
 H      -4.825448     3.138620     0.457074      28.37
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 H      -4.127646     4.109795    -0.755469      27.66
 H      -5.008742     2.595833    -1.160484      24.98
 C      -1.048735     1.214755     0.201297       1.66
 O      -0.210964     2.262417     0.972901     197.63
 C      -0.408334    -0.103397     0.204460      24.73
 H       0.578525    -0.195570     0.347641      22.07
 C      -2.620490    -1.097751    -0.295535      -3.54
 C      -3.593381    -2.183865    -0.714831      66.33
 H      -4.402832    -1.611042    -1.423249      20.29
 O      -2.886322    -3.178147    -1.534552     227.97
 H      -3.295541    -4.129190    -1.485543      16.93
 C      -4.298758    -2.773524     0.637400      88.95
 H      -3.458568    -3.154567     1.240507      23.16
 O      -5.098263    -1.996651     1.472762     356.62
 H      -4.688322    -1.168331     1.946619      25.84
 C      -5.299721    -4.067777     0.154460      89.99
 O      -4.714188    -5.214532    -0.624655     334.08
 H      -3.843531    -5.449328    -0.361075      29.95
 H      -5.997723    -3.593866    -0.595926      26.72
 H      -5.891603    -4.299796     0.880592      28.53
55
name = lig-etoh-frame_607
 C       2.061399     2.104875    -2.264488      54.64
 H       1.284263     2.664625    -2.874976      21.32
 C       3.046781     1.435043    -0.343668      46.26
 H       3.057994     1.561362     0.765874      19.10
 C       3.744436     0.313757    -0.852563      43.11
 O       4.136732    -0.750107    -0.079835     256.09
 C       5.417524    -0.556975     0.627129     115.74
 H       6.304887    -0.062544     0.172740      26.23
 H       5.847718    -1.479494     0.636959      27.13
 H       5.480098     0.002632     1.650902      25.72
 C       3.646220     0.079222    -2.236578       7.93
 O       4.133392    -1.002851    -3.081703     200.09
 H       4.538462    -1.664372    -2.415568      25.57
 C       2.750280     1.016403    -2.874062      49.44
 H       2.573320     0.688270    -3.761302      26.13
 C       2.236613     2.248205    -0.936525      53.53
 C       1.569695     3.430574    -0.164957     120.13
 H       1.769142     4.180097    -0.752454      28.14
 O       2.182176     3.500525     1.190925     274.46
 H       3.048717     4.031103     1.161594      28.69
 C       0.099081     3.364909     0.081822      87.20
 H      -0.527839     3.118034    -0.871270      22.08
 C      -0.376630     4.608162     0.774405     102.55
 O       0.062969     5.925587     0.169805     223.96
 H       0.238955     5.697375    -0.820351      29.02
 H       0.323060     4.664502     1.656527      23.85
 H      -1.497736     4.628985     0.670999      23.60
 C      -1.167522    -1.203514    -0.237127      62.51
 H      -0.507032    -2.171813    -0.493456      21.07
 C      -3.312102     0.202359    -0.137479      56.21
 H      -4.368375     0.491983    -0.396880      20.40
 C      -2.453607     1.343605     0.112105     -23.80
 O      -2.815878     2.774730     0.054969     131.66
 C      -4.252932     3.102881    -0.392937      99.32
 H      -4.967638     3.086028     0.661725      24.75
 H      -4.085159     4.156658    -0.980105      24.05
 H      -4.925534     2.779702    -1.135919      26.87
 C      -0.981990     1.195586     0.251023     -11.28
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 O      -0.257392     2.267913     0.943300     183.93
 C      -0.415084    -0.123532     0.204926      28.89
 H       0.779456    -0.082041     0.484846      20.05
 C      -2.551556    -1.050816    -0.245157      14.47
 C      -3.517443    -2.186379    -0.751593      83.22
 H      -4.172886    -1.843403    -1.454435      23.01
 O      -2.861648    -3.194935    -1.579355     228.45
 H      -3.407104    -4.122679    -1.401525      14.37
 C      -4.255358    -2.820043     0.561681      72.88
 H      -3.359622    -3.115060     1.215134      21.11
 O      -5.109735    -1.962853     1.464381     253.72
 H      -4.447314    -1.164824     1.915273      20.15
 C      -5.218707    -4.052677     0.109013      71.07
 O      -4.690067    -5.234967    -0.603798     260.82
 H      -3.868897    -5.692557    -0.115410      25.07
 H      -5.764801    -3.635941    -0.735078      26.20
 H      -6.156240    -4.237704     1.070985      23.65
55
name = lig-etoh-frame_608
 C       2.025295     2.060315    -2.307152      49.75
 H       1.352623     2.638640    -2.860299      24.11
 C       3.054470     1.378693    -0.263790      37.41
 H       3.094121     1.577721     0.789358      19.98
 C       3.723742     0.303253    -0.801199      35.79
 O       4.168785    -0.731004    -0.002172     262.86
 C       5.513393    -0.603234     0.602689      89.21
 H       6.311150    -0.021722     0.034831      24.58
 H       5.877856    -1.772660     0.890545      23.02
 H       5.394133    -0.068652     1.512015      26.22
 C       3.613172     0.074396    -2.266211       9.80
 O       4.151075    -0.953206    -3.025455     205.66
 H       4.389755    -1.683750    -2.421761      26.54
 C       2.712242     1.045792    -2.887477      48.55
 H       2.544668     0.801795    -4.139925      21.40
 C       2.285273     2.328666    -0.906428      41.32
 C       1.611478     3.333405    -0.247730      83.24
 H       1.477625     4.547490    -0.847321      17.99
 O       2.204560     3.519224     1.198490     225.75
 H       3.212789     3.723253     1.291501      26.71
 C       0.137925     3.359895     0.031324      82.77
 H      -0.357889     3.058392    -0.834881      24.90
 C      -0.392958     4.652660     0.698122     107.59
 O       0.058279     5.971540     0.122644     230.13
 H       0.194188     5.915767    -0.828217      30.81
 H       0.107048     4.577313     1.650833      26.25
 H      -1.459853     4.540695     0.798732      26.29
 C      -1.213006    -1.197993    -0.124256      70.73
 H      -0.886235    -2.035363    -0.596201      22.86
 C      -3.266985     0.233529    -0.047280      50.79
 H      -4.283899     0.431793    -0.314407      16.62
 C      -2.423573     1.272066     0.059198     -16.78
 O      -2.922015     2.794310    -0.013270     151.94
 C      -4.206768     3.080829    -0.363238     122.88
 H      -4.828829     3.222238     0.464226      28.07
 H      -4.096215     4.063398    -0.715824      27.39
 H      -4.607395     2.333898    -1.260498      24.83
 C      -0.943606     1.165258     0.359387      12.55
 O      -0.320399     2.232911     0.904419     185.78
 C      -0.380901    -0.066356     0.210531      52.48
 H       0.585208    -0.145692     0.454341      22.10
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 C      -2.563811    -1.020776    -0.257136      24.77
 C      -3.442945    -2.190694    -0.757663      74.85
 H      -4.303291    -1.753217    -1.489371      22.02
 O      -2.835209    -3.225451    -1.601680     272.62
 H      -3.371869    -3.931359    -1.427913      23.97
 C      -4.203331    -2.889113     0.501896      81.27
 H      -3.381918    -3.247336     1.092321      23.95
 O      -5.096165    -1.935912     1.413125     314.64
 H      -4.483819    -1.472758     1.900998      26.85
 C      -5.173685    -4.009085     0.079562     107.15
 O      -4.639270    -5.253708    -0.559500     296.82
 H      -4.157850    -5.782664     0.129771      29.86
 H      -5.706520    -3.589839    -0.804548      28.20
 H      -5.757215    -4.244158     0.790867      29.13
55
name = lig-etoh-frame_609
 C       2.003066     2.034862    -2.317586      62.66
 H       1.339356     2.774495    -2.963332      23.20
 C       3.083874     1.330054    -0.128261      47.46
 H       3.230368     1.439696     0.959443      20.24
 C       3.696166     0.257645    -0.824262      19.04
 O       4.226056    -0.724417     0.076254     268.02
 C       5.614611    -0.678501     0.596981      95.80
 H       6.140174    -0.162043    -0.206549      24.95
 H       5.798121    -1.585072     0.931882      27.11
 H       5.322775    -0.088992     1.546276      23.61
 C       3.544487     0.116406    -2.258480      16.15
 O       4.159065    -0.889128    -2.959208     182.32
 H       4.370923    -1.830672    -2.315829      20.91
 C       2.707556     0.997185    -2.995989      52.62
 H       2.552701     1.059905    -3.951510      24.96
 C       2.334273     2.349661    -0.979639      38.91
 C       1.643630     3.394103    -0.229985     106.68
 H       1.680710     4.248923    -0.715451      25.63
 O       2.229173     3.545217     1.187254     269.78
 H       3.167139     3.527358     1.125371      30.34
 C       0.136104     3.316596    -0.030041      54.87
 H      -0.269029     3.232248    -1.174743      22.21
 C      -0.381575     4.707176     0.620967      98.44
 O       0.046797     6.001952     0.080936     231.13
 H       0.006724     6.030743    -0.910675      29.58
 H      -0.207642     4.649282     1.782381      23.82
 H      -1.506031     4.572992     0.864167      24.13
 C      -1.244908    -1.164493    -0.024189      38.18
 H      -1.004617    -2.193806    -0.579952      20.44
 C      -3.200387     0.243590     0.013198      50.70
 H      -4.375821     0.203082    -0.166218      18.07
 C      -2.364911     1.322687     0.031676       1.22
 O      -2.944490     2.737905    -0.056876     152.10
 C      -4.195646     3.042382    -0.396294     105.60
 H      -5.056686     3.157678     0.600357      23.28
 H      -4.188926     4.186788    -0.744598      23.64
 H      -4.337984     2.220756    -1.011666      24.87
 C      -0.996354     1.157473     0.454301      29.53
 O      -0.360596     2.215951     0.888526     189.82
 C      -0.359796    -0.040461     0.218775      36.93
 H       0.791742    -0.282212     0.434946      20.58
 C      -2.632115    -1.018795    -0.289839      19.16
 C      -3.438856    -2.177968    -0.767929      85.26
 H      -4.242057    -1.675260    -1.202433      25.09
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 O      -2.788230    -3.227753    -1.608146     199.09
 H      -3.437019    -4.151665    -1.491078      16.53
 C      -4.151987    -2.928292     0.461043      80.39
 H      -3.370461    -3.489285     1.123293      21.83
 O      -5.063043    -1.955387     1.294726     233.65
 H      -4.402303    -1.612312     2.216951      20.46
 C      -5.112223    -3.957293    -0.019434      82.51
 O      -4.586056    -5.260889    -0.503762     246.53
 H      -4.322526    -5.763335     0.249118      30.31
 H      -5.845669    -3.543259    -0.747114      27.08
 H      -5.795762    -4.389390     1.057222      23.94
55
name = lig-etoh-frame_610
 C       2.011523     2.036078    -2.330586      62.77
 H       1.485154     2.715182    -2.869670      24.90
 C       3.099417     1.319323    -0.073727      46.11
 H       3.311331     1.296481     1.013442      19.98
 C       3.662706     0.221977    -0.809833       5.84
 O       4.264446    -0.742991     0.115110     217.02
 C       5.644860    -0.686932     0.601659      87.49
 H       6.269001    -0.384975    -0.313210      24.18
 H       5.975125    -1.862396     0.914565      22.94
 H       5.747201     0.007828     1.464127      25.49
 C       3.473467     0.145450    -2.234691      23.77
 O       4.173345    -0.861819    -2.888876     246.64
 H       4.388217    -1.502391    -2.330064      27.49
 C       2.695139     0.966959    -3.053855      45.83
 H       2.595017     1.028838    -4.298701      21.60
 C       2.398470     2.272463    -1.011387      14.58
 C       1.672724     3.466243    -0.117511      98.73
 H       2.106534     4.514368    -0.850079      19.81
 O       2.240264     3.574497     1.150750     268.54
 H       3.227975     3.502263     0.922224      25.89
 C       0.104215     3.302633    -0.108526      75.57
 H      -0.233760     3.330161    -1.063165      26.70
 C      -0.405196     4.733024     0.591194     100.01
 O       0.035544     6.017688     0.039144     209.61
 H      -0.285996     5.987914    -0.935428      28.69
 H      -0.123925     4.845044     1.586622      26.80
 H      -1.483629     4.748489     0.446559      25.69
 C      -1.267845    -1.159378     0.005064      52.70
 H      -0.781324    -2.096179    -0.137416      23.22
 C      -3.195758     0.215797     0.016247      54.66
 H      -4.209755     0.249887     0.063305      20.87
 C      -2.361268     1.438872     0.037834      18.20
 O      -2.845593     2.652002    -0.049466     192.38
 C      -4.265969     3.024654    -0.402041     115.76
 H      -4.913076     2.828630     0.339128      28.00
 H      -4.322256     3.947223    -1.001535      26.16
 H      -4.713916     2.181452    -1.147181      24.32
 C      -1.078377     1.161905     0.491758      19.89
 O      -0.351336     2.270178     0.884964     191.78
 C      -0.353369    -0.097750     0.247851      32.53
 H       0.724972    -0.185468     0.334564      22.71
 C      -2.639499    -1.018714    -0.288634      36.39
 C      -3.473517    -2.192796    -0.738182      70.47
 H      -4.411785    -1.686070    -1.273798      23.31
 O      -2.759552    -3.219871    -1.602083     261.37
 H      -3.171182    -4.063624    -1.567111      24.14
 C      -4.093706    -2.938608     0.454095     102.07
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 H      -3.444539    -3.483376     1.074096      25.25
 O      -4.973605    -1.996727     1.177439     358.39
 H      -4.710368    -1.751816     1.997292      33.52
 C      -5.127125    -3.975751    -0.052545     112.81
 O      -4.542690    -5.241347    -0.473472     281.53
 H      -4.298694    -5.746436     0.391169      29.17
 H      -5.915760    -3.602697    -0.701774      29.79
 H      -5.608293    -4.107739     0.751915      30.62
55
name = lig-etoh-frame_611
 C       2.084796     2.011216    -2.349379      60.96
 H       1.437301     2.872767    -2.860828      21.90
 C       3.113131     1.304305    -0.129820      54.74
 H       3.241283     1.378940     0.939345      21.11
 C       3.625470     0.222028    -0.731689      12.32
 O       4.289178    -0.771567     0.117257     235.66
 C       5.688094    -0.714555     0.582048     121.08
 H       6.372786    -0.443699    -0.159384      28.23
 H       5.964755    -1.634138     0.790658      29.25
 H       6.129125     0.059556     1.328066      26.36
 C       3.438453     0.117581    -2.215817      -2.54
 O       4.186040    -0.831231    -2.844654     133.63
 H       4.592411    -1.496016    -2.046378      19.55
 C       2.649699     0.991401    -3.098272      59.41
 H       2.765398     0.696419    -4.097775      25.85
 C       2.418106     2.201490    -0.917302      28.76
 C       1.731522     3.532321    -0.112634     111.75
 H       2.008107     4.352411    -0.601233      26.37
 O       2.263706     3.601138     1.123499     289.15
 H       3.269350     3.681347     1.005804      27.54
 C       0.110655     3.373452    -0.104689      59.02
 H      -0.407396     3.190194    -1.210610      22.88
 C      -0.455692     4.749618     0.535779      90.88
 O       0.025016     6.024699    -0.028102     224.10
 H      -0.391083     6.021588    -0.877358      30.48
 H       0.008893     4.857089     1.606167      23.73
 H      -1.516784     4.813625     0.166417      23.11
 C      -1.231302    -1.183508     0.002525      63.85
 H      -0.621732    -2.136400     0.206318      22.10
 C      -3.190347     0.229688    -0.025115      52.33
 H      -4.353849     0.437432     0.212971      17.61
 C      -2.416523     1.414726     0.077610      20.75
 O      -2.766171     2.647349    -0.041918     129.51
 C      -4.324851     2.917917    -0.472171      89.45
 H      -4.999052     2.705554     0.600755      22.22
 H      -4.328021     3.880668    -1.062345      24.90
 H      -4.863819     2.390810    -1.193284      26.01
 C      -1.081337     1.178331     0.479210       6.32
 O      -0.310765     2.357061     0.872856     178.55
 C      -0.439099    -0.121638     0.302162      38.82
 H       0.684712    -0.104734     0.337495      22.64
 C      -2.605272    -1.031745    -0.266031      33.45
 C      -3.528951    -2.220381    -0.711913      87.54
 H      -4.317946    -1.966729    -1.380725      24.91
 O      -2.722675    -3.162641    -1.590219     249.44
 H      -3.123691    -4.091992    -1.482149      21.15
 C      -4.081852    -2.937640     0.435290      93.44
 H      -3.276062    -3.437743     1.134006      22.94
 O      -4.896341    -2.045112     1.035822     303.47
 H      -4.670395    -1.737177     2.032847      26.46
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 C      -5.133911    -4.012204    -0.075302      57.53
 O      -4.518908    -5.217123    -0.456679     280.65
 H      -4.133496    -5.669155     0.330392      29.50
 H      -5.820829    -3.653942    -0.918360      26.83
 H      -5.883567    -4.021364     1.055087      24.33
55
name = lig-etoh-frame_612
 C       2.153434     2.048057    -2.336633      48.01
 H       1.548487     2.788484    -2.722461      22.44
 C       3.111120     1.317343    -0.166433      49.95
 H       3.144025     1.602790     0.910509      19.70
 C       3.621739     0.178474    -0.704870      15.52
 O       4.313075    -0.792665     0.096952     234.67
 C       5.740864    -0.694174     0.535082      83.43
 H       6.422539    -0.353175    -0.386701      25.36
 H       5.951867    -1.851798     0.920538      23.46
 H       6.031254     0.038015     1.357306      26.46
 C       3.427671     0.074372    -2.167814      -1.69
 O       4.208232    -0.842794    -2.795829     134.49
 H       4.826570    -1.297193    -2.042288      20.81
 C       2.651995     0.966128    -3.049183      51.21
 H       2.735730     0.535260    -4.139519      23.31
 C       2.356881     2.207795    -0.846165      48.96
 C       1.760981     3.490598    -0.192513      90.21
 H       1.873837     4.677115    -0.815842      20.65
 O       2.309343     3.632042     1.154568     286.88
 H       3.197017     3.977737     1.211437      30.29
 C       0.131526     3.480745    -0.093021      81.11
 H      -0.248783     3.119489    -0.945153      25.37
 C      -0.493988     4.773772     0.458800     111.04
 O       0.023267     6.028741    -0.103616     247.88
 H      -0.345020     6.159984    -1.021679      28.56
 H      -0.309291     4.681089     1.496234      27.17
 H      -1.588038     4.681599     0.430422      25.10
 C      -1.178113    -1.256234    -0.005676      52.68
 H      -0.780680    -2.269384     0.241994      22.86
 C      -3.231073     0.260261    -0.081081      56.41
 H      -4.230759     0.370427     0.016306      22.22
 C      -2.422261     1.287292     0.148784       1.99
 O      -2.778690     2.717249    -0.063301      72.62
 C      -4.369632     2.809371    -0.499109     103.51
 H      -4.772002     2.950768     0.452108      27.16
 H      -4.227461     3.949886    -0.671137      24.70
 H      -4.791372     2.116805    -1.367776      23.98
 C      -1.021071     1.221939     0.435152       9.91
 O      -0.270261     2.421775     0.854186     162.38
 C      -0.530954    -0.047047     0.381630      44.37
 H       0.637477    -0.132690     0.482735      22.36
 C      -2.597318    -1.064759    -0.239961       2.40
 C      -3.504878    -2.249159    -0.731839      82.69
 H      -4.358495    -1.956157    -1.445260      22.70
 O      -2.684252    -3.093120    -1.571795     210.34
 H      -3.090568    -4.083454    -1.301775      15.08
 C      -4.084035    -3.005047     0.414981     109.97
 H      -3.267197    -3.317152     1.004228      24.85
 O      -4.868966    -2.037017     0.950631     357.58
 H      -4.419221    -1.670957     1.893125      25.00
 C      -5.165543    -4.041160    -0.019037      96.87
 O      -4.513944    -5.210271    -0.455746     352.79
 H      -3.870648    -5.569162     0.163359      32.01
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 H      -5.556070    -3.716440    -0.974801      28.33
 H      -5.847962    -4.158150     0.652546      27.96
55
name = lig-etoh-frame_613
 C       2.207770     2.098944    -2.269999      44.92
 H       1.549696     2.880606    -2.839273      20.37
 C       3.094421     1.353548    -0.122949      32.67
 H       3.210182     1.646903     0.903247      18.54
 C       3.636542     0.124273    -0.725314       7.86
 O       4.336985    -0.808237     0.062899     259.81
 C       5.794724    -0.687181     0.465207     104.57
 H       6.273049    -0.431129    -0.392293      29.43
 H       5.944251    -1.613343     0.872512      27.96
 H       5.726102     0.009753     1.360832      26.82
 C       3.443238     0.027196    -2.097388      16.80
 O       4.249793    -0.882065    -2.755391     186.95
 H       4.854700    -1.231385    -2.186396      27.14
 C       2.704561     0.887479    -2.936817      53.71
 H       2.466769     0.758302    -4.050517      23.96
 C       2.259995     2.269973    -0.886926      57.17
 C       1.768744     3.494275    -0.276274     105.06
 H       1.879048     4.304821    -0.863324      27.46
 O       2.343213     3.664621     1.196233     235.13
 H       3.139052     4.344947     1.235470      26.87
 C       0.189098     3.555656    -0.068799      61.94
 H      -0.165148     3.157209    -1.168686      21.17
 C      -0.539178     4.797302     0.379548     106.83
 O       0.013691     6.030571    -0.169919     247.70
 H      -0.165973     6.154006    -1.173932      27.47
 H      -0.449172     4.742791     1.552785      23.95
 H      -1.637207     4.605202     0.534255      23.17
 C      -1.200122    -1.290635     0.004368      41.78
 H      -0.849784    -2.319321     0.047923      21.22
 C      -3.250302     0.199371    -0.148964      47.07
 H      -4.424019     0.241364    -0.331234      19.17
 C      -2.379565     1.299616     0.214469     -10.80
 O      -2.853243     2.735942    -0.096126     101.12
 C      -4.326683     2.769989    -0.516329     108.32
 H      -4.952442     2.820529     0.571589      24.52
 H      -4.326265     3.820580    -0.669521      25.72
 H      -4.528020     2.018380    -1.212306      26.38
 C      -0.970475     1.309167     0.387230       5.40
 O      -0.245161     2.443549     0.846248     169.86
 C      -0.525954    -0.008813     0.465349      36.27
 H       0.480658    -0.136654     0.717561      24.39
 C      -2.607173    -1.100821    -0.220915       1.87
 C      -3.444160    -2.254530    -0.797954      81.21
 H      -4.314092    -1.738951    -1.267944      23.23
 O      -2.643127    -3.059490    -1.549821     270.72
 H      -2.892803    -3.885523    -1.388458      23.22
 C      -4.108608    -3.082338     0.375257      89.66
 H      -3.229343    -3.446801     1.058735      21.26
 O      -4.874170    -1.967509     0.946067     383.80
 H      -4.391963    -1.567994     1.606132      31.67
 C      -5.132857    -4.063147    -0.002488      70.46
 O      -4.510148    -5.246787    -0.470986     309.19
 H      -3.552423    -5.464028    -0.053374      24.76
 H      -5.518603    -3.592463    -0.980191      24.35
 H      -6.225640    -4.396018     0.682916      22.48
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name = lig-etoh-frame_614
 C       2.225061     2.117928    -2.250746      45.11
 H       1.765187     2.766223    -2.991507      20.59
 C       3.060049     1.365234    -0.095529      41.68
 H       3.357145     1.560866     0.965872      19.10
 C       3.635576     0.159630    -0.681682      11.10
 O       4.350909    -0.834734     0.013548     251.35
 C       5.772041    -0.655999     0.412673      85.70
 H       6.452008    -0.324932    -0.502339      25.86
 H       6.132267    -1.717739     0.829112      24.22
 H       5.628542     0.160696     1.242511      25.12
 C       3.497018    -0.046410    -2.068232      17.25
 O       4.277253    -0.934656    -2.748524     127.12
 H       5.052132    -1.465327    -2.057010      19.54
 C       2.723159     0.877719    -2.786174      59.14
 H       2.429268     0.864021    -3.818908      25.50
 C       2.234326     2.284898    -0.917646      59.05
 C       1.736886     3.526484    -0.239577      92.18
 H       2.180301     4.400814    -1.160624      21.40
 O       2.371458     3.710998     1.206033     241.55
 H       2.967371     4.479061     1.081470      27.96
 C       0.234014     3.548862    -0.112462      76.98
 H      -0.076576     3.469628    -1.089947      23.68
 C      -0.574257     4.820584     0.366214     104.71
 O      -0.007579     6.036384    -0.234410     253.30
 H       0.024270     5.911230    -1.187787      30.95
 H      -0.267316     5.077036     1.361168      24.78
 H      -1.659176     4.682307     0.103779      23.75
 C      -1.263084    -1.225699     0.055209      40.39
 H      -0.704596    -2.230901    -0.198821      19.81
 C      -3.225924     0.126715    -0.195618      43.75
 H      -4.195219     0.179905    -0.643199      19.74
 C      -2.399004     1.406180     0.209661     -15.07
 O      -2.943807     2.696412    -0.117000     188.62
 C      -4.243851     2.781036    -0.431242     125.74
 H      -5.047522     2.319190     0.166759      27.17
 H      -4.627476     3.757256    -1.120882      23.91
 H      -4.423977     1.952506    -1.231300      25.79
 C      -0.953670     1.377173     0.363814     -14.70
 O      -0.224329     2.447101     0.839685     161.05
 C      -0.480263    -0.050219     0.517261       7.15
 H       0.620267    -0.159281     1.064079      21.56
 C      -2.612707    -1.124213    -0.220750      17.30
 C      -3.413508    -2.237967    -0.804957      81.95
 H      -4.249722    -1.707024    -1.314177      22.58
 O      -2.567082    -3.040530    -1.574704     196.07
 H      -2.832357    -4.093015    -1.532986      17.32
 C      -4.119421    -3.074513     0.383611      97.22
 H      -3.462137    -3.582345     1.056393      23.95
 O      -4.904568    -1.912445     0.956840     288.76
 H      -4.229600    -1.274681     1.655405      21.03
 C      -5.155240    -4.111987    -0.028931     102.20
 O      -4.487922    -5.315419    -0.498735     372.17
 H      -3.566462    -5.393442    -0.266158      29.78
 H      -5.690915    -3.577958    -0.806988      28.13
 H      -5.856324    -4.299279     0.590533      29.18
55
name = lig-etoh-frame_615
 C       2.231714     2.080046    -2.276981      46.93
 H       1.868949     2.749737    -3.058787      21.08
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 C       3.025952     1.345699    -0.087531      54.31
 H       3.322177     1.531128     0.932387      21.01
 C       3.633095     0.234981    -0.617975      18.61
 O       4.365357    -0.870252    -0.038282     254.13
 C       5.723724    -0.609710     0.364047     126.77
 H       6.356561    -0.113107    -0.311384      29.42
 H       6.226832    -1.507233     0.696597      28.16
 H       5.854144     0.209331     1.098757      28.35
 C       3.558170    -0.098249    -2.045627       6.16
 O       4.325674    -1.018267    -2.740980     229.34
 H       4.741816    -1.572105    -2.106763      26.23
 C       2.728078     0.899591    -2.657793      52.35
 H       2.608428     0.686101    -3.863262      22.88
 C       2.281004     2.275753    -0.841834      43.81
 C       1.752621     3.605469    -0.176969     110.16
 H       2.117090     4.336737    -0.780796      26.07
 O       2.372063     3.763796     1.165415     295.73
 H       2.980026     4.489016     1.035361      28.55
 C       0.237883     3.550723    -0.141306      57.34
 H      -0.185269     3.477970    -1.262614      20.79
 C      -0.562116     4.860824     0.349946      99.51
 O      -0.031736     6.046644    -0.317083     249.61
 H       0.222996     5.719719    -1.258054      28.45
 H      -0.339685     5.194131     1.404762      22.92
 H      -1.527262     4.782771    -0.150913      23.22
 C      -1.248878    -1.131376     0.131367      59.64
 H      -0.679908    -1.921841    -0.168753      23.48
 C      -3.137802     0.147730    -0.218777      44.63
 H      -4.085500     0.247539    -0.793259      20.67
 C      -2.454044     1.471267     0.126749      -1.49
 O      -2.976770     2.657480    -0.095265     226.15
 C      -4.274237     2.751084    -0.461448     143.72
 H      -5.053698     2.149626     0.172567      27.01
 H      -4.605375     3.489506    -1.020175      28.79
 H      -4.328387     2.110083    -1.343633      27.88
 C      -0.979599     1.352730     0.381031     -34.68
 O      -0.195557     2.453681     0.815498     142.32
 C      -0.433751    -0.072758     0.558332      38.86
 H       0.438999    -0.157562     0.994269      24.58
 C      -2.605401    -1.116731    -0.236960      27.90
 C      -3.415998    -2.251659    -0.760766      81.29
 H      -4.188697    -1.936217    -1.545481      21.83
 O      -2.471569    -3.058965    -1.628820     217.46
 H      -2.914799    -3.995878    -1.698389      19.75
 C      -4.153395    -2.990013     0.403654      82.11
 H      -3.507398    -3.571089     1.165044      20.74
 O      -4.921535    -1.870525     0.989509     363.77
 H      -4.408423    -1.411613     1.605447      30.49
 C      -5.140921    -4.136145    -0.108644      61.55
 O      -4.493956    -5.381433    -0.549776     302.40
 H      -3.520881    -5.450482    -0.231810      25.13
 H      -5.942439    -3.751973    -0.850839      24.94
 H      -5.769481    -4.352987     1.088392      23.71
55
name = lig-etoh-frame_616
 C       2.220642     2.057966    -2.228521      63.58
 H       1.808700     2.829330    -2.991293      19.94
 C       3.000780     1.329546    -0.046015      41.07
 H       3.133027     1.597652     1.016806      19.74
 C       3.667196     0.223059    -0.636443      30.56
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 O       4.382280    -0.891253    -0.063533     230.46
 C       5.684139    -0.522813     0.333235     105.09
 H       6.238315     0.037890    -0.568798      26.41
 H       6.213511    -1.466295     0.653668      26.14
 H       5.920322     0.173543     1.283616      25.69
 C       3.590026    -0.073582    -1.984274      12.60
 O       4.343642    -1.090011    -2.733657     201.21
 H       4.597509    -1.827151    -1.982056      22.70
 C       2.779462     0.827509    -2.675876      50.05
 H       2.815146     0.581997    -3.659852      25.10
 C       2.341417     2.302196    -0.774596      51.65
 C       1.791716     3.617391    -0.092410      93.29
 H       2.073123     4.784528    -0.702685      19.79
 O       2.343640     3.819580     1.116300     256.43
 H       3.223606     4.402161     1.134229      25.56
 C       0.185643     3.576985    -0.157987      69.49
 H      -0.126577     3.244627    -1.111730      21.86
 C      -0.505019     4.910714     0.311370     102.76
 O      -0.035744     6.061549    -0.420959     290.41
 H       0.336512     5.792054    -1.309037      27.13
 H      -0.728844     4.974360     1.417802      23.92
 H      -1.602126     4.754827     0.013173      23.17
 C      -1.200324    -1.072903     0.206301      38.02
 H      -0.558500    -2.076386     0.019021      18.93
 C      -3.071115     0.267132    -0.254825      56.98
 H      -4.095137     0.359817    -0.753750      20.56
 C      -2.430578     1.407774     0.022405      12.73
 O      -2.969388     2.672425    -0.043253     185.32
 C      -4.387845     2.631773    -0.564234      92.22
 H      -4.968884     2.311026     0.388022      25.52
 H      -4.599244     3.948070    -0.719791      22.87
 H      -4.361923     2.102311    -1.548667      24.79
 C      -1.034666     1.283650     0.434255     -20.24
 O      -0.171433     2.453233     0.772388     137.73
 C      -0.469679     0.014267     0.570189      47.16
 H       0.717936    -0.197156     0.913095      20.58
 C      -2.561868    -1.064857    -0.253153      31.33
 C      -3.400495    -2.291419    -0.750871      82.98
 H      -4.122827    -2.071264    -1.500514      22.78
 O      -2.396706    -3.092534    -1.664679     255.32
 H      -2.919703    -3.834305    -1.822929      24.10
 C      -4.200841    -2.908325     0.410350      83.80
 H      -3.505653    -3.295911     1.140433      22.07
 O      -4.958586    -1.868749     1.004856     354.89
 H      -4.403000    -1.455015     1.867180      23.10
 C      -5.151310    -4.159738    -0.099535     107.75
 O      -4.512491    -5.417028    -0.613800     326.60
 H      -3.649100    -5.636042    -0.093786      26.56
 H      -5.936899    -4.068869    -0.803374      27.35
 H      -5.452117    -4.363308     0.767040      29.52
55
name = lig-etoh-frame_617
 C       2.221420     2.026917    -2.135631      65.19
 H       1.744108     2.723936    -2.737281      22.89
 C       3.006430     1.310151     0.032189      62.18
 H       2.975522     1.512421     1.117614      21.43
 C       3.711053     0.157948    -0.643814      26.34
 O       4.385644    -0.889433    -0.047473     263.77
 C       5.706795    -0.420152     0.318490     107.28
 H       6.020160    -0.042455    -0.603450      27.95
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 H       6.190204    -1.440942     0.487904      25.73
 H       5.641205     0.109920     1.261799      26.58
 C       3.618093    -0.041100    -1.965359      13.71
 O       4.334516    -1.136481    -2.687967     164.30
 H       4.429103    -2.004495    -1.995690      21.09
 C       2.833038     0.773442    -2.742915      45.12
 H       2.876722     0.534473    -3.976749      21.80
 C       2.389173     2.358467    -0.778550      26.25
 C       1.817799     3.654426    -0.105886     108.96
 H       1.942461     4.545483    -0.713710      21.04
 O       2.327247     3.887759     1.141864     312.52
 H       3.304746     4.016262     1.136777      28.24
 C       0.154126     3.585278    -0.124913      58.67
 H      -0.075949     3.150313    -1.173364      19.74
 C      -0.506051     4.922482     0.242570     107.72
 O      -0.025474     6.089249    -0.498678     313.21
 H       0.249064     5.885026    -1.415110      26.76
 H      -0.649479     4.934614     1.329128      24.74
 H      -1.578120     4.724275     0.110184      23.94
 C      -1.164993    -1.124144     0.244535      38.13
 H      -0.708386    -2.022280     0.393361      21.82
 C      -3.089153     0.312664    -0.339515      56.70
 H      -4.082143     0.426841    -0.574492      19.72
 C      -2.318421     1.381290    -0.046846      19.24
 O      -2.976443     2.693291    -0.005334     100.83
 C      -4.471738     2.616423    -0.638841     111.13
 H      -5.054695     2.315758     0.230949      25.62
 H      -4.549785     3.558243    -0.430077      27.40
 H      -4.632607     2.119515    -1.624506      24.59
 C      -1.066985     1.290042     0.493333      21.63
 O      -0.172518     2.430257     0.738360     149.42
 C      -0.454507     0.119408     0.596044      55.39
 H       0.525214     0.020477     0.659445      23.93
 C      -2.486788    -0.987800    -0.265953      22.25
 C      -3.331104    -2.292873    -0.774966      64.53
 H      -4.192897    -1.895006    -1.480602      21.14
 O      -2.350642    -3.119028    -1.650775     199.52
 H      -3.010660    -3.957048    -2.020271      18.62
 C      -4.229404    -2.872193     0.383194      79.08
 H      -3.458963    -3.202547     1.150643      20.68
 O      -5.001181    -1.860195     1.026186     330.62
 H      -4.589951    -1.660560     1.992411      24.87
 C      -5.112634    -4.189462    -0.083844      74.18
 O      -4.528594    -5.425562    -0.676431     275.93
 H      -3.851975    -5.794698    -0.112263      28.73
 H      -5.999944    -4.068419    -0.823133      24.99
 H      -5.661984    -4.623032     1.085748      23.70
55
name = lig-etoh-frame_618
 C       2.262568     1.945273    -2.079383      44.79
 H       1.565561     2.684128    -2.709920      20.28
 C       3.041063     1.280638     0.078271      78.49
 H       2.990332     1.274512     1.166187      21.90
 C       3.703783     0.137975    -0.569213      13.02
 O       4.374032    -0.885826     0.003201     237.66
 C       5.729462    -0.385366     0.305345      84.86
 H       6.159962     0.192779    -0.593526      26.61
 H       6.290628    -1.259951     0.471297      27.01
 H       5.447693     0.321834     1.254370      24.25
 C       3.655633    -0.057860    -2.044227       4.53
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 O       4.296665    -1.166003    -2.614851     245.53
 H       4.385444    -1.845577    -2.092202      28.79
 C       2.854654     0.801311    -2.846202      34.87
 H       2.757382     0.681635    -3.805661      23.92
 C       2.446317     2.366788    -0.766031      59.60
 C       1.793235     3.651723    -0.159994      87.66
 H       1.985561     4.497186    -1.127762      18.08
 O       2.317585     3.952508     1.215466     312.37
 H       3.295590     3.770572     1.095494      25.73
 C       0.170527     3.542622    -0.112037      66.97
 H      -0.034760     3.383297    -1.189682      19.13
 C      -0.546008     4.904342     0.169699      91.27
 O      -0.011670     6.115027    -0.534725     223.97
 H      -0.036190     5.920860    -1.591043      24.49
 H      -0.125852     5.224115     1.235187      20.87
 H      -1.651165     4.784700    -0.088190      21.95
 C      -1.152021    -1.127439     0.283196      44.06
 H      -0.771864    -2.165161     0.675528      19.40
 C      -3.094571     0.273158    -0.440318      44.59
 H      -4.285363     0.409851    -0.450800      17.53
 C      -2.276586     1.461318    -0.090218       6.74
 O      -3.001108     2.675796    -0.004371      80.80
 C      -4.494507     2.610353    -0.644748      73.82
 H      -5.296758     1.884892    -0.023184      22.28
 H      -4.725972     3.900834    -0.481880      21.81
 H      -4.793225     2.278998    -1.642042      23.86
 C      -1.033767     1.405460     0.529148      32.28
 O      -0.189948     2.407942     0.735866     187.67
 C      -0.449317     0.106316     0.605742      11.27
 H       0.783710     0.256679     0.635956      18.86
 C      -2.426417    -0.960285    -0.290692      22.43
 C      -3.266510    -2.220130    -0.828802      75.66
 H      -3.955068    -1.740105    -1.451659      23.27
 O      -2.364089    -3.154870    -1.604211     286.69
 H      -2.852058    -3.873861    -1.964290      24.50
 C      -4.205224    -2.903576     0.361744      86.64
 H      -3.509914    -3.303813     1.107747      22.49
 O      -5.055840    -1.860161     1.037939     369.12
 H      -4.740856    -1.719141     1.882971      30.84
 C      -5.115180    -4.255902    -0.002614     112.62
 O      -4.555493    -5.400052    -0.742605     322.58
 H      -3.858427    -5.901079    -0.151618      26.46
 H      -5.849958    -3.804301    -0.636368      29.13
 H      -5.640804    -4.534638     0.738225      30.31
55
name = lig-etoh-frame_619
 C       2.297317     1.885774    -2.103053      38.27
 H       1.653144     2.447042    -2.643841      23.75
 C       3.096723     1.242492     0.085301      66.59
 H       3.098211     1.126822     1.196257      21.18
 C       3.639804     0.164813    -0.553871      16.55
 O       4.379362    -0.887791     0.072384     249.65
 C       5.725081    -0.333799     0.304738     109.54
 H       6.224204     0.371713    -0.362078      28.22
 H       6.520411    -1.136435     0.713773      26.18
 H       5.690222     0.380401     1.051500      29.21
 C       3.669742    -0.073628    -2.105047       0.03
 O       4.245846    -1.160041    -2.573735     148.36
 H       4.497523    -1.948713    -1.740575      17.33
 C       2.876825     0.871879    -2.847660      54.56
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 H       2.510608     0.797981    -4.061687      19.79
 C       2.507271     2.297524    -0.707045      52.76
 C       1.754882     3.631648    -0.222482      86.65
 H       2.018396     4.387347    -0.991334      20.83
 O       2.292240     4.004740     1.251141     287.98
 H       3.303849     3.787296     1.186636      25.14
 C       0.222674     3.511233    -0.147025      69.85
 H      -0.095617     3.373487    -1.222738      20.15
 C      -0.548336     4.917432     0.137676     105.78
 O      -0.006222     6.116247    -0.582971     241.85
 H      -0.208338     6.065324    -1.509406      28.75
 H      -0.112995     5.324173     0.977138      23.25
 H      -1.595814     4.877111    -0.042696      24.30
 C      -1.127313    -1.086021     0.338343      59.09
 H      -0.888703    -2.105330     0.587473      19.70
 C      -3.044269     0.268830    -0.506810      47.26
 H      -4.049665     0.209542    -0.526797      21.17
 C      -2.352935     1.525966    -0.122647       1.17
 O      -3.069577     2.652040    -0.043847     164.88
 C      -4.524413     2.658820    -0.595319     115.45
 H      -5.133458     1.885929    -0.208554      26.09
 H      -4.879285     3.544448    -0.643423      28.23
 H      -4.503147     2.503594    -1.745160      24.67
 C      -0.998313     1.458856     0.498976      10.03
 O      -0.176357     2.445900     0.766886     193.17
 C      -0.409294     0.067401     0.602750      29.38
 H       0.601129     0.218965     0.844816      19.63
 C      -2.404019    -0.996996    -0.328668      20.69
 C      -3.213981    -2.146599    -0.851261      63.90
 H      -3.871081    -1.626791    -1.700599      19.10
 O      -2.390958    -3.163708    -1.528707     243.98
 H      -2.959733    -3.955192    -1.794257      20.39
 C      -4.152207    -2.964680     0.360785      71.35
 H      -3.435872    -3.353026     1.122555      20.58
 O      -5.111759    -1.893490     0.996256     276.87
 H      -4.671991    -1.610437     2.038832      20.66
 C      -5.095518    -4.263597     0.015175      75.02
 O      -4.589479    -5.357182    -0.797180     292.88
 H      -3.824007    -5.780741    -0.338650      27.93
 H      -5.789886    -3.624452    -0.635136      25.60
 H      -5.855106    -4.632292     1.072023      24.35
55
name = lig-etoh-frame_620
 C       2.337094     1.884581    -2.093231      68.75
 H       1.583715     2.538424    -2.746484      23.02
 C       3.143325     1.226530     0.102957      56.70
 H       3.241988     1.226176     1.167493      21.31
 C       3.601346     0.140125    -0.648222      19.06
 O       4.404647    -0.869153     0.140043     221.47
 C       5.751818    -0.290169     0.349503      99.46
 H       6.139433     0.269400    -0.567908      28.12
 H       6.402311    -0.959837     0.745649      28.76
 H       5.812630     0.542417     1.261838      25.69
 C       3.633382    -0.039334    -2.078178      15.62
 O       4.209051    -1.201832    -2.536804     214.84
 H       4.623548    -1.498841    -1.714156      18.63
 C       2.906571     0.900599    -2.862547      34.90
 H       2.540950     0.836518    -3.770500      21.90
 C       2.528168     2.198595    -0.674069      48.44
 C       1.753900     3.555896    -0.214068      85.51
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 H       2.139194     4.601375    -0.843392      18.55
 O       2.247292     4.035429     1.236870     283.18
 H       3.204990     4.075227     1.281018      27.87
 C       0.254425     3.521193    -0.224118      67.82
 H      -0.175406     3.061038    -1.180493      20.09
 C      -0.486516     4.953398     0.104652      83.47
 O      -0.008943     6.109464    -0.621963     275.74
 H      -0.196580     6.113491    -1.640169      25.89
 H      -0.399128     5.206843     1.311191      22.11
 H      -1.659348     4.848393     0.154045      21.94
 C      -1.145365    -1.054792     0.359553      48.42
 H      -0.774949    -2.091007     0.422487      19.10
 C      -2.920558     0.283932    -0.537419      53.68
 H      -4.075840     0.109656    -0.833346      20.93
 C      -2.430828     1.509070    -0.126778       3.59
 O      -3.181221     2.674935    -0.092785     191.41
 C      -4.480718     2.681743    -0.606543      98.03
 H      -5.136811     1.704277    -0.123548      22.75
 H      -5.126845     3.779585    -0.477315      22.80
 H      -4.118136     2.570672    -1.608944      24.53
 C      -1.017107     1.399521     0.392919     -29.21
 O      -0.135719     2.535383     0.820428     121.47
 C      -0.401832     0.107895     0.605640      24.35
 H       0.669888    -0.025053     1.151936      17.17
 C      -2.372767    -1.010830    -0.352838      29.27
 C      -3.215519    -2.122200    -0.872245      78.00
 H      -3.823937    -1.792891    -1.636174      22.05
 O      -2.416129    -3.168861    -1.451712     192.52
 H      -3.165999    -3.987077    -1.428690      13.75
 C      -4.101257    -3.001056     0.384923      68.44
 H      -3.277912    -3.221223     1.125010      20.23
 O      -5.129228    -1.959265     0.960566     349.31
 H      -4.734346    -1.533344     1.663858      28.00
 C      -5.115132    -4.214469     0.032466     106.83
 O      -4.625715    -5.298734    -0.840965     355.95
 H      -3.741994    -5.609262    -0.516816      29.60
 H      -5.862686    -3.819988    -0.631753      27.76
 H      -5.498464    -4.526232     0.842873      28.45
55
name = lig-etoh-frame_621
 C       2.342006     1.962117    -2.073740      69.95
 H       1.757220     2.648763    -2.584053      23.82
 C       3.181961     1.215670     0.099700      44.00
 H       3.420475     1.413486     1.184772      20.04
 C       3.619131     0.077673    -0.707871      18.12
 O       4.434416    -0.825034     0.185991     209.34
 C       5.772210    -0.194566     0.419566      97.56
 H       5.996691    -0.062845    -0.658821      26.72
 H       6.422633    -1.184320     0.728194      24.96
 H       5.684748     0.483548     1.139749      28.37
 C       3.582568    -0.022353    -2.032442      36.04
 O       4.176231    -1.226549    -2.510998     206.15
 H       4.809310    -1.451610    -1.686151      18.96
 C       2.945566     0.904542    -2.823190      49.73
 H       2.611204     0.706579    -3.999603      19.53
 C       2.484866     2.148371    -0.684586      32.44
 C       1.842197     3.509169    -0.160825     103.16
 H       2.128910     4.370914    -0.763319      22.79
 O       2.171181     4.039592     1.196841     263.87
 H       3.152698     4.397039     1.177240      25.68
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 C       0.239629     3.536323    -0.286049      65.95
 H      -0.090670     2.989557    -1.146826      20.83
 C      -0.435505     4.979518     0.120134     103.34
 O      -0.018994     6.108693    -0.635889     339.68
 H       0.016469     5.864817    -1.639646      26.11
 H      -0.441253     4.982259     1.134584      26.17
 H      -1.471108     4.746769     0.024539      23.89
 C      -1.175993    -1.066083     0.342800      36.52
 H      -0.477950    -1.998977     0.317472      18.92
 C      -2.878903     0.268436    -0.579733      59.71
 H      -3.734136     0.316530    -1.193375      23.28
 C      -2.450281     1.480019    -0.101342      -3.37
 O      -3.237944     2.718552    -0.091065     176.02
 C      -4.473693     2.689947    -0.645811     129.81
 H      -5.041750     1.917737    -0.270779      28.21
 H      -4.766773     3.571348    -0.279700      26.99
 H      -4.320911     2.540465    -1.794530      25.30
 C      -1.017565     1.370389     0.295333     -23.89
 O      -0.131296     2.603366     0.868114      59.82
 C      -0.406039     0.176385     0.622633      27.38
 H       0.419131    -0.128870     1.284981      19.06
 C      -2.332134    -0.983406    -0.361499      35.87
 C      -3.237473    -2.167181    -0.844330      67.39
 H      -4.101109    -1.820966    -1.612709      20.22
 O      -2.451048    -3.201642    -1.375739     268.43
 H      -2.981692    -3.893256    -1.304079      23.01
 C      -4.082921    -2.955742     0.399672      79.65
 H      -3.276714    -3.166590     1.099319      21.32
 O      -5.123889    -2.061378     0.897981     328.10
 H      -4.651893    -1.368646     1.584021      23.28
 C      -5.088682    -4.125321    -0.020797      74.16
 O      -4.644803    -5.234640    -0.876250     302.45
 H      -3.672450    -5.522859    -0.639666      25.59
 H      -6.073857    -3.869124    -0.528811      24.53
 H      -5.359915    -4.655119     1.186637      21.91
55
name = lig-etoh-frame_622
 C       2.354281     2.034245    -2.078205      65.98
 H       1.827177     2.930862    -2.600604      19.40
 C       3.211119     1.199837     0.047851      49.61
 H       3.545477     1.473000     1.028677      20.15
 C       3.673155     0.060971    -0.579901      16.23
 O       4.445612    -0.779460     0.205790     251.38
 C       5.782249    -0.206096     0.445306     101.50
 H       6.198189     0.041340    -0.538366      29.55
 H       6.301079    -1.010218     0.780362      28.24
 H       5.643748     0.776923     1.180215      24.77
 C       3.562385    -0.094175    -2.032464      14.57
 O       4.141191    -1.227526    -2.489917     125.47
 H       4.948462    -1.731607    -1.881159      18.99
 C       2.927548     0.930425    -2.801085      56.06
 H       2.971556     0.671395    -3.833939      23.05
 C       2.423908     2.148722    -0.673057      50.08
 C       1.914884     3.479071    -0.095507      86.47
 H       2.285009     4.208766    -1.095791      20.93
 O       2.105057     4.024450     1.150070     283.89
 H       2.941960     4.547302     1.032606      25.42
 C       0.253880     3.550597    -0.269363      49.05
 H      -0.022132     3.122270    -1.344384      18.14
 C      -0.402320     4.930884     0.088081      81.30
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 O      -0.016284     6.109780    -0.622845     310.68
 H       0.209636     5.730203    -1.517935      27.97
 H      -0.113828     5.050325     1.277414      21.04
 H      -1.477086     4.695217    -0.324021      20.01
 C      -1.115186    -1.066682     0.316206      55.78
 H      -0.512815    -1.881755     0.354016      20.62
 C      -2.902076     0.276732    -0.650443      54.84
 H      -3.653080     0.453326    -1.513524      21.80
 C      -2.405541     1.490863    -0.064459      -5.19
 O      -3.180865     2.719680    -0.053822     138.01
 C      -4.476418     2.685396    -0.749566     101.82
 H      -5.310804     1.809373    -0.276237      23.55
 H      -4.803070     3.781561    -0.243674      22.95
 H      -4.806884     2.676393    -1.801366      25.77
 C      -0.996534     1.445073     0.275189     -18.90
 O      -0.181720     2.633610     0.878111     101.32
 C      -0.478715     0.172943     0.633111      27.14
 H       0.425028     0.181345     1.271343      20.68
 C      -2.345449    -0.992805    -0.391049      20.33
 C      -3.300262    -2.219836    -0.786347      81.73
 H      -4.064839    -1.849235    -1.373726      23.10
 O      -2.453527    -3.228893    -1.321909     245.81
 H      -2.945350    -4.207392    -1.353194      12.61
 C      -4.096668    -2.856218     0.365856      99.92
 H      -3.368776    -3.301382     1.159744      20.80
 O      -5.098034    -2.147258     0.861853     336.17
 H      -4.721005    -1.286279     1.409727      24.32
 C      -5.050080    -4.092498    -0.023140     106.18
 O      -4.639631    -5.161952    -0.914131     377.83
 H      -3.810719    -5.529021    -0.628766      32.35
 H      -6.043518    -3.704141    -0.242574      28.02
 H      -5.196352    -4.457065     0.828179      29.72
55
name = lig-etoh-frame_623
 C       2.358099     2.098149    -2.107546      55.44
 H       2.056259     2.974869    -2.695330      21.00
 C       3.208451     1.225631    -0.008494      51.88
 H       3.580044     1.466604     1.014786      18.95
 C       3.720696     0.075124    -0.464004      17.38
 O       4.470974    -0.754455     0.223104     277.96
 C       5.765334    -0.202259     0.461223     112.49
 H       6.420077     0.304909    -0.332234      27.51
 H       6.417387    -0.991802     1.131264      25.17
 H       5.749449     0.592586     1.091182      29.81
 C       3.555429    -0.165904    -1.956494       2.76
 O       4.123173    -1.257151    -2.512446     196.23
 H       4.709801    -1.755502    -2.085136      24.67
 C       2.919105     0.934770    -2.738864      46.33
 H       3.132993     0.836903    -3.908385      22.22
 C       2.394680     2.153291    -0.648706      50.22
 C       1.903614     3.470519    -0.138704     105.03
 H       2.352725     4.134397    -0.947621      21.15
 O       2.069421     4.013703     1.121975     302.14
 H       2.871175     4.532249     1.144007      28.15
 C       0.320734     3.548154    -0.237425      65.15
 H       0.023611     3.343971    -1.206165      21.27
 C      -0.385652     4.849032     0.063652     110.05
 O       0.011020     6.106194    -0.583706     297.90
 H       0.329986     5.918670    -1.592447      27.01
 H      -0.145776     5.163579     0.983977      24.72
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 H      -1.402202     4.757355    -0.171492      24.81
 C      -1.053582    -1.028683     0.271182      51.88
 H      -0.581926    -2.118947     0.504963      17.37
 C      -2.938885     0.314037    -0.724281      40.69
 H      -3.658812     0.426648    -1.572097      21.23
 C      -2.338886     1.522270    -0.061601       2.42
 O      -3.091862     2.677578    -0.044706     104.55
 C      -4.553369     2.710229    -0.777734     112.91
 H      -5.136499     2.019782    -0.359949      28.86
 H      -4.965975     3.642745    -0.525952      27.55
 H      -4.798119     2.809994    -1.887872      26.15
 C      -0.986803     1.562549     0.335649       5.76
 O      -0.275607     2.629493     0.835396     180.83
 C      -0.545855     0.163629     0.645411      28.42
 H       0.497692     0.556373     1.039644      18.31
 C      -2.398325    -1.023881    -0.429003       1.97
 C      -3.321277    -2.257842    -0.711333      73.65
 H      -4.116839    -1.798060    -1.508281      19.46
 O      -2.444184    -3.273295    -1.291584     260.53
 H      -2.896339    -4.193375    -1.504399      14.10
 C      -4.074565    -2.841272     0.322542     124.31
 H      -3.476816    -3.284485     1.084358      21.11
 O      -5.112728    -2.143980     0.874866     402.42
 H      -4.850008    -1.418386     1.275021      34.52
 C      -4.987593    -4.063864    -0.049404      70.07
 O      -4.633219    -5.081719    -0.965958     319.91
 H      -3.922577    -5.632521    -0.477735      29.80
 H      -5.944842    -3.541456    -0.278174      26.42
 H      -5.156822    -4.607877     1.172989      24.76
55
name = lig-etoh-frame_624
 C       2.387588     2.104436    -2.119533      60.51
 H       2.175219     2.943236    -2.808640      17.86
 C       3.190867     1.301315     0.022050      54.92
 H       3.419161     1.506341     1.065069      17.04
 C       3.721621     0.089651    -0.506994      22.09
 O       4.537478    -0.767802     0.260599     295.11
 C       5.809602    -0.220230     0.517173     113.53
 H       6.311648     0.216698    -0.318032      28.69
 H       6.352784    -0.837170     1.157209      27.41
 H       5.661500     0.692612     1.341029      25.40
 C       3.539253    -0.180053    -1.823234      22.67
 O       4.082399    -1.279443    -2.587664     119.33
 H       4.730126    -1.964375    -1.861208      19.44
 C       2.939652     0.899022    -2.667803      58.45
 H       3.123652     1.125850    -3.758247      25.70
 C       2.391561     2.164308    -0.682851      54.09
 C       1.823335     3.480675    -0.209656     103.40
 H       2.378558     4.424537    -0.802422      19.63
 O       2.060061     4.005156     1.138606     255.18
 H       3.029031     4.359809     1.335277      28.46
 C       0.386884     3.539395    -0.214672      64.87
 H      -0.048048     3.220490    -1.295499      18.22
 C      -0.363254     4.819369     0.038418      88.33
 O       0.070623     6.103937    -0.559858     295.23
 H       0.127206     6.116921    -1.500024      30.73
 H      -0.318234     5.169896     1.215845      22.49
 H      -1.533523     4.675554     0.094018      21.48
 C      -1.066292    -1.043406     0.205172      38.85
 H      -0.775054    -1.941264     0.564362      19.50
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 C      -2.922302     0.321538    -0.754899      44.58
 H      -3.792114     0.419745    -1.428526      21.57
 C      -2.315035     1.541341    -0.129267       3.59
 O      -3.044182     2.655226    -0.072321      84.80
 C      -4.589204     2.766046    -0.807519      62.16
 H      -5.182305     1.752996    -0.204294      21.32
 H      -4.978571     3.806812    -0.488291      23.70
 H      -4.313154     2.663845    -1.885277      24.42
 C      -1.029929     1.584295     0.416774      24.14
 O      -0.360419     2.634569     0.774789     205.85
 C      -0.530998     0.262994     0.649307      28.59
 H       0.497503     0.278243     0.906798      19.76
 C      -2.437381    -1.003201    -0.446442       3.42
 C      -3.289341    -2.237020    -0.754960      95.99
 H      -3.928112    -1.973596    -1.519614      20.96
 O      -2.420175    -3.312751    -1.282743     286.08
 H      -2.991010    -4.014736    -1.526072      18.76
 C      -4.069040    -2.919015     0.341801      97.79
 H      -3.258318    -3.185927     1.163967      19.83
 O      -5.171303    -2.096518     0.907256     278.47
 H      -4.780412    -1.171128     1.449080      22.22
 C      -4.952769    -4.068201    -0.010030     119.49
 O      -4.608542    -5.012540    -1.018782     381.86
 H      -4.114871    -5.721115    -0.483682      31.53
 H      -5.841547    -3.629191    -0.502223      27.45
 H      -5.155289    -4.488071     0.803665      29.38
55
name = lig-etoh-frame_625
 C       2.444407     2.038126    -2.119210      30.79
 H       2.154897     2.879452    -2.854280      17.06
 C       3.171605     1.356816     0.095361     100.00
 H       3.205072     1.574817     1.172158      16.79
 C       3.724791     0.121045    -0.520634      29.41
 O       4.590408    -0.800379     0.292336     239.80
 C       5.848645    -0.180004     0.627215      95.69
 H       6.235153     0.047318    -0.437793      25.05
 H       6.500945    -1.044507     1.157408      24.63
 H       5.613341     0.665858     1.204942      29.14
 C       3.517442    -0.186639    -1.818647      18.22
 O       4.049559    -1.301297    -2.619578     218.18
 H       4.471501    -1.825008    -1.984089      28.35
 C       2.966676     0.885567    -2.584679      74.02
 H       3.136192     0.953595    -3.678575      25.07
 C       2.403234     2.222591    -0.748274      53.75
 C       1.805981     3.547619    -0.222806     104.88
 H       2.100033     4.421686    -0.888142      21.81
 O       2.079919     3.987365     1.192681     311.12
 H       3.060361     3.953994     1.261452      30.76
 C       0.321589     3.514520    -0.274465      77.28
 H       0.076310     3.066515    -1.152000      22.45
 C      -0.373025     4.876593     0.094788     104.00
 O       0.134738     6.097000    -0.520130     279.26
 H      -0.166559     6.035977    -1.543535      26.66
 H      -0.298265     4.902741     1.119163      27.71
 H      -1.387575     4.568435    -0.044699      24.34
 C      -1.167324    -0.987216     0.140116      27.43
 H      -0.728294    -1.975671     0.636310      18.69
 C      -2.876130     0.321455    -0.752278      61.06
 H      -3.991198     0.431002    -1.096170      21.51
 C      -2.358796     1.512347    -0.250744       8.73
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 O      -3.053152     2.688039    -0.118381     131.60
 C      -4.564410     2.767116    -0.793777      95.80
 H      -5.069142     2.045716    -0.464208      29.53
 H      -4.755774     3.842220    -0.453042      24.31
 H      -4.042256     2.495777    -1.697126      24.35
 C      -1.098148     1.493406     0.467267      27.06
 O      -0.398054     2.690810     0.743774     198.68
 C      -0.479126     0.312955     0.619596      26.67
 H       0.557207    -0.115018     0.961210      17.63
 C      -2.421153    -0.949056    -0.440967      27.43
 C      -3.219388    -2.221429    -0.840020      69.93
 H      -3.998354    -2.021021    -1.731966      17.96
 O      -2.376060    -3.330862    -1.283391     208.77
 H      -3.246130    -4.006717    -1.583394      12.90
 C      -4.050637    -2.953835     0.430974      89.13
 H      -3.283256    -3.087844     1.117086      21.99
 O      -5.212980    -2.011845     0.954998     301.23
 H      -4.701812    -1.363812     1.518777      24.54
 C      -4.957364    -4.062662    -0.036114      92.91
 O      -4.560918    -4.977000    -1.069101     329.06
 H      -4.161597    -5.754603    -0.737378      33.96
 H      -5.830775    -3.644302    -0.533509      26.40
 H      -5.433820    -4.718764     1.046439      22.49
55
name = lig-etoh-frame_626
 C       2.481628     2.003490    -2.120928      60.27
 H       2.105397     2.694044    -2.786716      23.92
 C       3.138406     1.377378     0.133879      63.02
 H       3.078773     1.559644     1.224179      19.02
 C       3.755462     0.158210    -0.421084      15.82
 O       4.595345    -0.827558     0.309132     214.71
 C       5.890583    -0.172563     0.695803     103.19
 H       6.351513     0.007979    -0.269204      26.65
 H       6.513153    -0.992166     1.056066      26.62
 H       5.742790     0.818889     1.274647      27.16
 C       3.509860    -0.204663    -1.905980      16.64
 O       3.992186    -1.282424    -2.625521     203.34
 H       4.488806    -1.946180    -1.946691      23.19
 C       3.011280     0.844610    -2.571496      56.71
 H       3.095685     0.443247    -3.698821      19.50
 C       2.453056     2.311362    -0.745078      17.83
 C       1.809423     3.612565    -0.178831      76.01
 H       1.805965     4.411717    -1.111711      19.36
 O       2.122335     3.946342     1.224986     335.01
 H       3.081704     3.737572     1.217567      26.96
 C       0.196532     3.496116    -0.327747      44.80
 H       0.024455     2.969658    -1.406463      17.59
 C      -0.379885     4.917747     0.129751      84.09
 O       0.181792     6.082087    -0.487230     250.14
 H      -0.217167     5.888891    -1.370522      27.83
 H      -0.135130     4.855601     1.284708      23.28
 H      -1.443787     4.754350    -0.336690      20.12
 C      -1.225487    -0.906957     0.149485      53.74
 H      -0.731673    -1.824171     0.392843      19.36
 C      -2.917347     0.344552    -0.749373      65.50
 H      -3.935521     0.337358    -0.874031      20.87
 C      -2.402213     1.493189    -0.334090       8.38
 O      -3.091363     2.733575    -0.165520     173.86
 C      -4.406592     2.789048    -0.771743      97.08
 H      -5.439346     1.934510    -0.418510      21.32
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 H      -4.680890     3.794501    -0.604169      25.01
 H      -4.243820     2.569653    -1.906999      23.64
 C      -1.130466     1.447152     0.465068     -14.94
 O      -0.430313     2.737787     0.746776     158.97
 C      -0.430518     0.205306     0.563773      28.95
 H       0.482237     0.063465     1.055176      16.78
 C      -2.396457    -0.936483    -0.461237      35.49
 C      -3.179586    -2.226003    -0.914159      77.26
 H      -3.903398    -1.960426    -1.622203      20.77
 O      -2.359474    -3.339555    -1.305953     273.88
 H      -2.930040    -4.005497    -1.534970      20.34
 C      -4.069713    -2.894773     0.480935      58.92
 H      -3.264357    -3.154907     1.335334      19.52
 O      -5.205866    -1.948361     0.999061     306.34
 H      -4.703241    -1.442528     1.686698      24.68
 C      -5.016676    -4.110535    -0.016439     103.45
 O      -4.507046    -4.949620    -1.130549     324.79
 H      -3.986035    -5.789769    -0.883876      31.72
 H      -5.875377    -3.488880    -0.409721      27.65
 H      -5.423944    -4.596320     0.681638      28.09
55
name = lig-etoh-frame_627
 C       2.500404     2.017913    -2.097550      62.56
 H       1.939532     2.687074    -2.925190      21.66
 C       3.109280     1.359913     0.141426      48.01
 H       3.118514     1.491979     1.214126      20.29
 C       3.776375     0.165823    -0.350409      24.38
 O       4.579632    -0.813888     0.326738     229.47
 C       5.909536    -0.183006     0.718476      97.29
 H       6.474523     0.182966    -0.168686      25.63
 H       6.531956    -0.962507     1.278730      25.71
 H       5.929979     0.713819     1.454461      26.60
 C       3.557537    -0.217969    -1.861825      14.90
 O       3.937589    -1.271245    -2.605108     192.65
 H       4.561271    -2.020421    -2.044523      22.46
 C       3.041873     0.761431    -2.674497      46.18
 H       2.895109     0.415591    -3.652910      21.61
 C       2.533651     2.388569    -0.698613      18.50
 C       1.754266     3.635107    -0.167030      87.94
 H       1.926999     4.475016    -0.912505      19.83
 O       2.171179     3.895827     1.213455     317.85
 H       3.202830     3.788784     1.323939      25.32
 C       0.104482     3.481144    -0.357920      67.05
 H      -0.143357     3.239335    -1.328028      21.94
 C      -0.407511     4.914376     0.135270     103.45
 O       0.224324     6.064232    -0.452139     260.95
 H       0.035635     5.998692    -1.410745      29.95
 H      -0.234412     5.016119     1.190103      25.15
 H      -1.432592     5.160042    -0.118629      23.47
 C      -1.183212    -0.890514     0.200534      54.55
 H      -0.692321    -1.926676     0.189720      17.42
 C      -3.032134     0.326376    -0.756746      40.23
 H      -4.219163     0.262770    -0.960208      17.11
 C      -2.380568     1.544387    -0.318359       3.00
 O      -3.123250     2.752133    -0.214367     235.48
 C      -4.293568     2.774311    -0.788536     143.96
 H      -5.035858     2.317229    -0.396693      29.21
 H      -4.779941     3.871692    -0.771774      24.44
 H      -4.565422     2.730926    -1.869471      25.81
 C      -1.115095     1.453825     0.397344     -10.23
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 O      -0.484881     2.726236     0.762379     175.94
 C      -0.440924     0.143146     0.510327      35.51
 H       0.522710     0.308423     1.108553      15.57
 C      -2.419291    -0.944451    -0.536973      23.60
 C      -3.155731    -2.245864    -0.895937      63.03
 H      -3.965486    -1.876339    -1.675928      18.66
 O      -2.319592    -3.306753    -1.341477     227.19
 H      -2.865491    -4.222555    -1.529792      11.89
 C      -4.115569    -2.813867     0.504975      75.86
 H      -3.507739    -3.131946     1.260351      23.39
 O      -5.145607    -1.905186     1.028631     300.46
 H      -4.819130    -1.450728     2.039822      21.30
 C      -5.042598    -4.103038    -0.044837      76.38
 O      -4.463540    -4.922765    -1.192078     283.01
 H      -3.810390    -5.589055    -0.775797      28.62
 H      -5.849855    -3.512085    -0.427027      27.60
 H      -5.548008    -4.907567     0.916927      24.19
55
name = lig-etoh-frame_628
 C       2.512845     2.027685    -2.109252      46.52
 H       1.978753     2.603864    -2.747017      24.76
 C       3.110163     1.322081     0.144217      55.25
 H       3.236498     1.468661     1.246530      21.34
 C       3.771543     0.149358    -0.369601      28.93
 O       4.577362    -0.757095     0.362120     258.73
 C       5.926798    -0.218691     0.743081      96.47
 H       6.413236     0.276674    -0.134492      25.33
 H       6.431205    -0.987923     1.417960      24.89
 H       5.772210     0.543374     1.473566      27.50
 C       3.629372    -0.180751    -1.736073      26.35
 O       3.916972    -1.313019    -2.565315     263.84
 H       4.482935    -1.857358    -2.182632      30.76
 C       3.024016     0.751127    -2.733144      17.90
 H       2.588943     0.590416    -3.876462      19.33
 C       2.603499     2.412202    -0.690174      18.55
 C       1.700669     3.603136    -0.180153     105.03
 H       2.219285     4.627353    -0.544909      16.18
 O       2.205713     3.844749     1.196639     310.18
 H       3.152468     4.026017     1.219325      28.40
 C       0.060027     3.535533    -0.292579      65.91
 H      -0.376478     3.359365    -1.391771      19.70
 C      -0.454336     4.932439     0.109745      99.47
 O       0.283052     6.059338    -0.428003     236.75
 H       0.430287     6.125896    -1.465908      27.97
 H      -0.320951     5.083600     1.241045      24.03
 H      -1.593995     5.188642     0.206391      23.23
 C      -1.149487    -1.013181     0.198329      28.44
 H      -0.642263    -2.028177     0.124449      16.41
 C      -3.171244     0.293569    -0.746898      47.41
 H      -4.098138     0.345337    -1.154234      18.55
 C      -2.370944     1.568059    -0.262196       0.37
 O      -3.062575     2.756780    -0.249673     177.73
 C      -4.311384     2.855931    -0.879686      91.95
 H      -5.082108     2.182312     0.064483      20.46
 H      -4.599739     3.843793    -0.711978      25.57
 H      -4.478769     2.574636    -1.980284      24.50
 C      -1.091061     1.483834     0.283628      23.87
 O      -0.548467     2.661338     0.766782     200.03
 C      -0.454163     0.237393     0.501303      27.75
 H       0.553929     0.272440     0.992823      16.78
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 C      -2.438690    -0.927239    -0.598490      11.92
 C      -3.189588    -2.254414    -0.836068      83.73
 H      -3.891952    -2.040875    -1.619891      21.78
 O      -2.267152    -3.263252    -1.388180     224.64
 H      -2.915567    -4.090158    -1.423370      13.91
 C      -4.191183    -2.755622     0.478989      69.05
 H      -3.413270    -3.150348     1.299910      21.69
 O      -5.065870    -1.859422     1.073175     382.21
 H      -4.861834    -1.566348     1.857930      32.23
 C      -5.057254    -4.095676    -0.048667     104.53
 O      -4.424824    -4.891656    -1.216749     359.98
 H      -3.761883    -5.326634    -0.695420      30.70
 H      -5.982884    -3.702893    -0.583793      27.20
 H      -5.264341    -4.724664     0.634844      28.91
55
name = lig-etoh-frame_629
 C       2.549848     1.991120    -2.122047      64.38
 H       1.907905     2.793799    -2.747840      21.60
 C       3.141831     1.312074     0.149493      58.73
 H       3.297449     1.485276     1.196556      24.39
 C       3.770257     0.135062    -0.408837      28.32
 O       4.578529    -0.700002     0.407974     282.83
 C       5.905056    -0.254274     0.779594      91.87
 H       6.386258     0.121360    -0.102930      26.78
 H       6.407406    -1.108809     1.241508      25.48
 H       5.504540     0.636337     1.497147      23.37
 C       3.664223    -0.119661    -1.744387      23.75
 O       3.899068    -1.349056    -2.500856     173.89
 H       4.761060    -2.006633    -2.037507      18.54
 C       2.958054     0.820525    -2.697604      21.76
 H       2.667232     0.643289    -3.627225      24.34
 C       2.629988     2.354896    -0.725786      64.68
 C       1.725964     3.572589    -0.178083      97.69
 H       2.047707     4.473814    -0.625770      18.67
 O       2.201903     3.788372     1.204871     277.87
 H       3.108675     4.251003     0.981035      24.93
 C       0.031044     3.622009    -0.213257      71.37
 H      -0.337298     3.305595    -1.152908      21.55
 C      -0.512107     4.999326     0.129590     105.34
 O       0.351843     6.074948    -0.411622     253.46
 H       0.528299     5.922810    -1.345528      30.61
 H      -0.176492     5.023707     1.206242      23.99
 H      -1.613836     4.919577     0.107081      24.73
 C      -1.137752    -1.090829     0.132370      20.30
 H      -0.603803    -2.030858     0.227093      17.44
 C      -3.192252     0.298535    -0.693846      63.25
 H      -4.135691     0.447767    -1.417980      16.43
 C      -2.454988     1.505134    -0.246069      -1.03
 O      -2.954059     2.774637    -0.291727     159.37
 C      -4.407425     2.898617    -0.906739      95.40
 H      -4.924969     2.354559    -0.290921      29.99
 H      -4.477122     4.072731    -0.691968      23.67
 H      -4.272884     2.380551    -1.880677      25.89
 C      -1.080284     1.499974     0.171027      19.52
 O      -0.586353     2.609677     0.756881     183.75
 C      -0.486210     0.289173     0.489922      21.38
 H       0.532145     0.196964     0.845124      19.69
 C      -2.447400    -0.921867    -0.592739      13.06
 C      -3.241043    -2.238771    -0.779951      77.06
 H      -4.003569    -2.168585    -1.662668      19.87
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 O      -2.230624    -3.210999    -1.413670     235.46
 H      -2.852476    -3.901639    -1.514973      19.18
 C      -4.205086    -2.772898     0.441626      71.63
 H      -3.450651    -3.108197     1.060182      24.02
 O      -5.016803    -1.815450     1.070104     319.67
 H      -4.534826    -1.450607     2.070801      20.72
 C      -5.053611    -4.019355    -0.130713      87.30
 O      -4.389038    -4.846634    -1.197762     324.29
 H      -3.597212    -5.343773    -0.706488      25.90
 H      -6.054851    -3.907103    -0.532783      25.47
 H      -5.159305    -4.888380     0.890438      23.64
55
name = lig-etoh-frame_630
 C       2.537992     2.036631    -2.124456      42.85
 H       2.075111     2.738453    -2.709935      20.42
 C       3.196772     1.331108     0.125336      38.03
 H       3.274519     1.545169     1.216552      19.99
 C       3.794655     0.149036    -0.409927       9.98
 O       4.547193    -0.679884     0.439806     257.09
 C       5.828841    -0.246532     0.826052     110.22
 H       6.466310    -0.004419    -0.119312      28.13
 H       6.427360    -1.228327     1.113466      25.32
 H       5.831803     0.580033     1.409577      29.96
 C       3.656249    -0.089803    -1.886844      21.09
 O       3.918903    -1.386829    -2.398516     190.64
 H       4.654315    -1.812179    -1.981859      23.98
 C       2.928364     0.859776    -2.578129      63.45
 H       2.804824     0.467803    -3.745206      22.59
 C       2.603360     2.252263    -0.750655      41.66
 C       1.766882     3.519576    -0.150774      78.51
 H       1.785397     4.371858    -1.085183      20.67
 O       2.189189     3.743643     1.203518     262.72
 H       3.021369     4.322384     1.082679      25.76
 C       0.046251     3.657017    -0.135760      60.60
 H      -0.222157     3.233101    -1.184895      19.30
 C      -0.510819     5.055558     0.198427     102.99
 O       0.396945     6.090298    -0.396535     225.00
 H       0.439184     5.710809    -1.326022      29.58
 H      -0.234186     5.108436     1.257997      24.54
 H      -1.595865     4.963925    -0.197068      22.94
 C      -1.159701    -1.032190     0.032808      39.83
 H      -0.612988    -2.026176     0.396242      19.06
 C      -3.153456     0.334117    -0.649041      71.82
 H      -3.944715     0.352846    -1.313185      22.15
 C      -2.556029     1.426094    -0.266380       2.46
 O      -2.881573     2.801277    -0.347047     136.16
 C      -4.402621     2.980599    -0.912869      82.77
 H      -5.354859     2.198354    -0.283365      22.59
 H      -4.575863     3.985642    -1.016256      26.10
 H      -4.214100     2.445791    -1.911598      24.84
 C      -1.108225     1.462482     0.092742      -8.79
 O      -0.590273     2.612981     0.745571     148.59
 C      -0.538471     0.215416     0.438968      27.92
 H       0.599120     0.230606     0.783516      20.52
 C      -2.454617    -0.963711    -0.519788      21.40
 C      -3.298820    -2.199659    -0.797132      82.13
 H      -4.039820    -2.082682    -1.598762      21.25
 O      -2.212988    -3.141040    -1.405078     166.98
 H      -2.830334    -3.988714    -1.844766      15.18
 C      -4.177422    -2.815957     0.365301      72.69
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 H      -3.382315    -3.309864     1.115042      20.32
 O      -4.969723    -1.760104     1.089591     347.26
 H      -4.308031    -1.389842     1.693597      26.62
 C      -5.034597    -4.008717    -0.156016     110.59
 O      -4.342184    -4.796342    -1.151802     388.97
 H      -3.628695    -5.373417    -0.832317      31.97
 H      -6.106306    -3.848700    -0.425114      27.11
 H      -5.108419    -4.500044     0.662119      29.27
55
name = lig-etoh-frame_631
 C       2.498217     2.132852    -2.094163      59.15
 H       2.078285     2.878698    -2.888912      19.05
 C       3.271200     1.337341     0.095425      45.60
 H       3.224561     1.583394     1.148180      18.55
 C       3.827073     0.194200    -0.437155       8.72
 O       4.481642    -0.681990     0.459358     257.58
 C       5.806998    -0.270353     0.815371     119.14
 H       6.333606    -0.027861    -0.057207      30.36
 H       6.255780    -1.098357     1.257531      28.57
 H       6.187730     0.616933     1.520722      26.99
 C       3.659024    -0.113916    -1.927262      16.55
 O       3.927505    -1.395088    -2.311256     190.90
 H       4.745864    -1.748355    -1.759636      21.55
 C       2.934042     0.800560    -2.582554      72.32
 H       2.900348     0.577350    -3.558196      26.99
 C       2.512774     2.201643    -0.729362      42.22
 C       1.768184     3.459870    -0.160830      96.90
 H       1.901849     4.117531    -0.945616      24.67
 O       2.175932     3.731928     1.184422     288.18
 H       3.024834     4.157846     1.363142      29.95
 C       0.103382     3.597717    -0.095263      64.39
 H      -0.083922     3.459976    -1.184567      19.38
 C      -0.459899     5.084403     0.270060      95.42
 O       0.414775     6.089090    -0.390368     221.43
 H       0.343815     5.770608    -1.389464      28.18
 H      -0.673982     5.338142     1.397751      24.13
 H      -1.374179     5.317758    -0.317929      23.53
 C      -1.181701    -0.964461    -0.036782      70.33
 H      -0.806883    -1.826674     0.302412      22.20
 C      -3.118292     0.264778    -0.637375      48.82
 H      -4.120317     0.234112    -1.194156      21.39
 C      -2.533472     1.485459    -0.270800       3.35
 O      -2.896669     2.822719    -0.413646     191.17
 C      -4.365821     2.982378    -0.910930     118.45
 H      -5.146555     2.594163    -0.463064      29.62
 H      -4.724454     4.096831    -1.231259      24.66
 H      -4.373231     2.666890    -1.951326      26.93
 C      -1.162382     1.388927     0.085256      -5.68
 O      -0.585124     2.629088     0.728001     161.57
 C      -0.556051     0.143099     0.352008      55.74
 H       0.372579     0.209307     0.734499      22.20
 C      -2.495398    -0.992874    -0.424897      32.07
 C      -3.321815    -2.174986    -0.852911      73.11
 H      -4.072338    -1.822815    -1.652405      20.18
 O      -2.236718    -3.086103    -1.399364     272.81
 H      -2.629047    -3.731909    -1.905433      23.87
 C      -4.108053    -2.845124     0.307870      95.20
 H      -3.540416    -3.350041     1.013019      21.37
 O      -4.911364    -1.739603     1.066499     324.22
 H      -4.196611    -1.235514     1.594520      25.05
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 C      -5.008445    -3.986655    -0.171593      77.12
 O      -4.309640    -4.751401    -1.126144     363.28
 H      -3.675638    -5.356417    -0.695131      29.28
 H      -5.996077    -3.604914    -0.513693      27.02
 H      -5.212957    -4.631900     0.993019      24.09
55
name = lig-etoh-frame_632
 C       2.465720     2.146838    -2.107789      46.64
 H       2.086891     2.899107    -2.820849      17.46
 C       3.312470     1.354288     0.061524      62.57
 H       3.305738     1.535736     1.141520      17.49
 C       3.864070     0.235307    -0.489056      16.67
 O       4.410868    -0.677858     0.475049     256.92
 C       5.828290    -0.300687     0.795408      87.68
 H       6.318274    -0.085998    -0.240916      26.48
 H       6.171542    -1.217413     1.498235      24.62
 H       5.894200     0.568518     1.454002      27.59
 C       3.672851    -0.154341    -1.812622      10.75
 O       3.948896    -1.412322    -2.246064     174.95
 H       4.782020    -1.751503    -1.545959      18.97
 C       2.934550     0.805529    -2.644936      55.49
 H       2.824410     0.684839    -3.851424      24.11
 C       2.391290     2.216100    -0.685227      49.96
 C       1.741894     3.387966    -0.135630      94.49
 H       2.278052     4.342841    -0.799332      19.99
 O       2.150707     3.737563     1.182783     240.87
 H       3.192546     3.856978     1.379959      28.21
 C       0.178139     3.534843    -0.077604      68.30
 H      -0.142800     3.598519    -1.175327      18.58
 C      -0.395635     5.111412     0.308780     109.92
 O       0.433927     6.082416    -0.385744     259.63
 H       0.311809     6.007248    -1.304270      32.83
 H      -0.845684     5.374378     1.200400      27.15
 H      -1.343191     5.338943    -0.234653      24.46
 C      -1.217008    -0.983297    -0.075952      44.26
 H      -0.733269    -2.075172     0.168723      17.27
 C      -3.138698     0.196980    -0.654589      63.53
 H      -4.237167     0.203246    -0.840221      23.37
 C      -2.459003     1.571622    -0.293373       0.87
 O      -2.985346     2.845819    -0.488099     200.90
 C      -4.273089     3.031047    -0.984199     101.65
 H      -5.250340     2.659292    -0.089210      23.47
 H      -4.475538     4.088129    -0.996265      25.39
 H      -4.546547     2.606306    -2.051287      24.67
 C      -1.197493     1.369942     0.145466      19.10
 O      -0.583344     2.614790     0.700102     177.47
 C      -0.550617     0.170354     0.252298      47.76
 H       0.508625     0.095968     0.854541      17.42
 C      -2.581927    -0.974568    -0.364721      32.89
 C      -3.308807    -2.175210    -0.912383      82.65
 H      -3.981075    -1.677106    -1.660917      19.83
 O      -2.266971    -3.013844    -1.396293     250.28
 H      -2.743784    -3.755849    -1.952987      18.24
 C      -4.064235    -2.825897     0.273287      87.75
 H      -3.289482    -3.306031     1.036861      18.92
 O      -4.841863    -1.764229     0.997509     314.28
 H      -4.234939    -1.090467     1.679385      20.49
 C      -5.005717    -3.967723    -0.103125     108.58
 O      -4.288406    -4.731132    -1.115688     362.47
 H      -3.683718    -5.306050    -0.484822      26.84
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 H      -5.808711    -3.497011    -0.689497      28.38
 H      -5.367430    -4.535539     0.586641      29.59
55
name = lig-etoh-frame_633
 C       2.448233     2.044645    -2.130101      49.84
 H       2.009753     2.877976    -2.724276      14.69
 C       3.274703     1.428089     0.031148     101.33
 H       3.485769     1.428984     1.125043      18.86
 C       3.907607     0.255108    -0.493006      26.43
 O       4.364238    -0.666358     0.478912     269.32
 C       5.826046    -0.365368     0.775686     100.64
 H       6.384769    -0.307618    -0.113038      27.48
 H       6.169180    -1.130148     1.342538      28.34
 H       5.597053     0.651472     1.305024      25.48
 C       3.634963    -0.155543    -1.737782       9.49
 O       3.998299    -1.441887    -2.175211     240.54
 H       4.549549    -1.841833    -1.648459      29.73
 C       2.945774     0.863149    -2.716685      66.60
 H       2.801967     0.710547    -3.757691      24.32
 C       2.334440     2.203232    -0.675061      63.12
 C       1.736005     3.420274    -0.083981     117.88
 H       2.127222     4.224517    -0.566321      26.04
 O       2.143137     3.740347     1.230997     299.40
 H       3.074501     3.580661     1.062405      29.17
 C       0.223312     3.529553    -0.099223      60.08
 H      -0.253280     3.509335    -1.129917      19.69
 C      -0.343276     5.109332     0.259874      89.67
 O       0.471838     6.094528    -0.349763     230.30
 H       0.209209     6.106222    -1.358246      28.02
 H      -0.596572     5.389546     1.400402      25.10
 H      -1.382184     4.896675    -0.217086      23.30
 C      -1.227318    -1.081761    -0.071168      32.74
 H      -0.709632    -1.946332    -0.106852      17.53
 C      -3.202725     0.293490    -0.639697      55.16
 H      -4.281958     0.278153    -0.654851      22.82
 C      -2.469012     1.563309    -0.368926       2.39
 O      -3.046388     2.854181    -0.554430     218.18
 C      -4.269400     3.068377    -1.029935     116.53
 H      -4.867782     2.727555    -0.229149      26.49
 H      -4.189921     4.253051    -0.863609      22.27
 H      -4.535408     2.521729    -1.898592      26.24
 C      -1.176943     1.459346     0.231916      13.48
 O      -0.576426     2.575533     0.683545     228.31
 C      -0.492390     0.182098     0.193529      25.99
 H       0.382736     0.076740     0.657601      17.77
 C      -2.630876    -0.967980    -0.350715      17.84
 C      -3.291671    -2.166921    -0.932050      81.43
 H      -3.979612    -1.851289    -1.756547      20.17
 O      -2.294245    -2.965861    -1.435338     221.72
 H      -2.916465    -3.832663    -1.714258      14.44
 C      -4.017507    -2.791369     0.311235     103.37
 H      -3.114888    -3.056867     0.813381      22.99
 O      -4.776623    -1.796468     0.915218     426.88
 H      -4.393161    -1.426196     1.632350      31.98
 C      -5.004506    -3.894199    -0.107492      74.31
 O      -4.264978    -4.746417    -1.085568     337.96
 H      -3.619133    -5.264971    -0.608936      29.34
 H      -5.755637    -3.429937    -0.803029      25.86
 H      -5.686232    -4.701995     0.694852      22.61
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name = lig-etoh-frame_634
 C       2.403833     1.929294    -2.131554      56.68
 H       1.875669     2.765278    -2.726633      20.75
 C       3.229725     1.477861     0.030635      60.63
 H       3.476523     1.560267     1.072116      20.23
 C       3.914242     0.293522    -0.443897      41.15
 O       4.349417    -0.663079     0.467841     266.91
 C       5.762042    -0.408616     0.760460      89.68
 H       6.485624    -0.460769    -0.136868      25.38
 H       6.266904    -1.223431     1.480783      24.97
 H       5.769532     0.701548     1.105674      26.12
 C       3.575371    -0.150616    -1.777195      -2.81
 O       4.015655    -1.440505    -2.142052     144.50
 H       4.621994    -2.104004    -1.425131      21.75
 C       2.991016     0.886325    -2.714244      60.94
 H       2.865094     0.629889    -3.827125      19.91
 C       2.351807     2.170400    -0.697972      26.24
 C       1.692359     3.467730    -0.021983      89.03
 H       1.926565     4.443583    -0.848045      17.80
 O       2.153208     3.725937     1.300692     283.38
 H       3.131970     3.553922     1.136813      25.27
 C       0.208374     3.569410    -0.144529      65.59
 H      -0.112758     3.313088    -1.172356      20.50
 C      -0.318945     5.038450     0.221283     112.93
 O       0.500057     6.117640    -0.327325     202.54
 H       0.223117     6.117148    -1.294296      28.62
 H      -0.074700     5.183333     1.219312      26.25
 H      -1.279691     4.805815    -0.144214      24.45
 C      -1.239004    -1.084512    -0.055344      32.70
 H      -0.601262    -2.061589    -0.314347      16.01
 C      -3.254933     0.444229    -0.580960      53.97
 H      -4.411075     0.461884    -0.693349      18.92
 C      -2.529089     1.518890    -0.447146      11.62
 O      -2.984335     2.822817    -0.596111     200.76
 C      -4.319095     3.148052    -1.055771      95.47
 H      -5.082249     2.664457    -0.112753      21.44
 H      -4.297394     4.249661    -1.194947      24.31
 H      -4.565103     2.557100    -2.041988      23.56
 C      -1.150855     1.508170     0.259382       4.46
 O      -0.538950     2.570418     0.706940     183.07
 C      -0.503722     0.162421     0.151082       5.41
 H       0.669925     0.120456     0.518587      15.64
 C      -2.615754    -0.929820    -0.391562      11.62
 C      -3.315598    -2.128130    -0.928918      75.85
 H      -4.096305    -2.079558    -1.771639      18.81
 O      -2.313649    -2.982252    -1.504058     233.44
 H      -2.844672    -3.775311    -1.483003      17.88
 C      -3.972758    -2.776084     0.331901      92.02
 H      -3.010184    -3.072326     0.905382      21.08
 O      -4.752585    -1.814441     0.833486     339.94
 H      -4.402843    -1.663363     1.935586      21.24
 C      -5.011297    -3.867729    -0.133637      97.25
 O      -4.249245    -4.776891    -1.053685     387.26
 H      -3.498444    -5.326773    -0.647816      29.43
 H      -5.742426    -3.360549    -0.739208      29.46
 H      -5.538351    -4.311682     0.562499      27.99
55
name = lig-etoh-frame_635
 C       2.301748     1.893550    -2.104390      72.30
 H       1.804418     2.502385    -2.802167      24.20
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 C       3.240170     1.452256     0.081735      26.59
 H       3.305654     1.883418     1.129954      17.88
 C       3.845853     0.333085    -0.441015      30.52
 O       4.363958    -0.662965     0.455162     263.44
 C       5.737219    -0.455511     0.745159     112.82
 H       6.290800    -0.618849    -0.163698      26.46
 H       6.012590    -1.022549     1.577085      27.72
 H       6.073104     0.619316     1.084133      26.32
 C       3.565991    -0.144212    -1.803761      10.67
 O       4.017043    -1.432800    -2.133853     211.69
 H       4.498286    -1.830198    -1.328336      22.06
 C       3.067912     0.799942    -2.698754      55.08
 H       2.996891     0.582402    -3.828648      20.07
 C       2.365912     2.203403    -0.741827      25.07
 C       1.665521     3.522618    -0.037545     104.05
 H       1.855551     4.274788    -0.713200      23.23
 O       2.175320     3.703192     1.350801     284.89
 H       3.192340     3.818664     1.512854      27.78
 C       0.170716     3.600491    -0.202028      80.06
 H       0.140268     3.146774    -1.275584      20.41
 C      -0.259735     4.926961     0.188743      86.16
 O       0.501381     6.134473    -0.330279     197.06
 H       0.388360     6.162112    -1.272926      30.13
 H       0.156094     4.900567     1.284801      23.84
 H      -1.460727     5.210858     0.061979      22.43
 C      -1.243365    -1.023473    -0.066050      54.28
 H      -0.781646    -1.949802    -0.321814      18.36
 C      -3.336037     0.453847    -0.515038      56.07
 H      -4.300373     0.617777    -0.839446      18.84
 C      -2.507893     1.567015    -0.454197       8.61
 O      -2.899835     2.811835    -0.642116     165.90
 C      -4.391626     3.169570    -1.066375     106.51
 H      -5.188338     2.930445    -0.391925      26.25
 H      -4.540276     4.295051    -1.438870      24.40
 H      -4.590680     2.777025    -2.017573      26.46
 C      -1.158892     1.427791     0.192583       1.80
 O      -0.478623     2.612814     0.761831     140.48
 C      -0.513394     0.171716     0.161622      40.75
 H       0.522790     0.183712     0.194733      19.27
 C      -2.590493    -0.830303    -0.477623       8.05
 C      -3.345535    -2.103115    -0.930083      75.07
 H      -4.187780    -1.954629    -1.592582      22.06
 O      -2.322594    -3.015307    -1.581736     171.66
 H      -2.766688    -4.023361    -1.362733      11.75
 C      -3.911540    -2.818218     0.296958     108.00
 H      -3.263453    -3.240450     1.077576      23.12
 O      -4.759403    -1.782304     0.837675     357.05
 H      -4.621396    -1.644069     1.761184      29.53
 C      -4.933869    -3.841785    -0.193901      69.89
 O      -4.249013    -4.822664    -1.027973     322.59
 H      -3.552644    -5.349340    -0.457989      27.67
 H      -5.715504    -3.281012    -0.795666      28.03
 H      -5.553242    -4.295443     0.898503      25.51
55
name = lig-etoh-frame_636
 C       2.224598     1.855709    -2.098847      79.36
 H       1.600395     2.363236    -2.976529      22.86
 C       3.234205     1.451965     0.143168      17.43
 H       3.252657     1.905267     1.095422      19.93
 C       3.747838     0.323130    -0.446185      16.40
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 O       4.374986    -0.641809     0.436647     253.39
 C       5.738847    -0.480026     0.729905     100.13
 H       6.274676    -0.893723    -0.189606      24.61
 H       5.820389    -1.108238     1.727172      24.67
 H       6.217219     0.547509     0.993265      25.55
 C       3.614266    -0.150278    -1.783042      16.70
 O       3.997945    -1.395280    -2.138804     233.38
 H       4.423166    -1.625586    -1.281883      21.43
 C       3.099520     0.719248    -2.679554      53.23
 H       3.093543     0.535898    -3.728190      21.12
 C       2.373692     2.275536    -0.761075      40.05
 C       1.706612     3.514954    -0.063747      98.84
 H       2.229935     4.529084    -0.664937      19.27
 O       2.183012     3.686213     1.386794     265.37
 H       3.027427     4.148051     1.450125      28.61
 C       0.156421     3.534915    -0.271845      95.69
 H       0.039192     3.246631    -1.269425      23.44
 C      -0.237867     4.912057     0.198458     110.71
 O       0.488355     6.131436    -0.333083     192.43
 H       0.532795     6.118467    -1.386626      27.32
 H      -0.010054     4.785166     1.224697      26.92
 H      -1.134402     5.343499     0.365021      26.69
 C      -1.278572    -0.913816    -0.112772      52.66
 H      -0.863774    -1.952249    -0.243697      19.33
 C      -3.353687     0.403080    -0.469942      49.11
 H      -4.365026     0.590179    -1.049750      16.65
 C      -2.448265     1.605680    -0.386658       3.70
 O      -2.870954     2.878636    -0.704151     113.50
 C      -4.407095     3.194543    -1.109059      80.67
 H      -5.432381     3.076277    -0.333379      22.97
 H      -4.455179     4.318474    -1.352573      24.65
 H      -4.609697     2.631846    -2.121061      23.60
 C      -1.173979     1.378719     0.100366      13.61
 O      -0.434263     2.638285     0.791949     103.89
 C      -0.530335     0.196229     0.182851      55.40
 H       0.622404     0.197265     0.117322      19.88
 C      -2.606851    -0.742885    -0.574077      20.88
 C      -3.308519    -2.098995    -0.925281      58.92
 H      -4.260131    -1.685782    -1.485387      22.62
 O      -2.352219    -3.058500    -1.644239     234.56
 H      -2.619258    -3.922709    -1.547272      20.69
 C      -3.899510    -2.844816     0.266819      99.74
 H      -3.351783    -3.340970     1.097674      23.12
 O      -4.796604    -1.745121     0.836943     295.16
 H      -4.586665    -1.465108     1.868239      24.20
 C      -4.867541    -3.847221    -0.202904     117.18
 O      -4.256413    -4.890015    -0.989871     378.26
 H      -3.777391    -5.365953    -0.349550      33.91
 H      -5.581612    -3.408237    -0.848099      31.53
 H      -5.265230    -4.195124     0.610400      31.59
55
name = lig-etoh-frame_637
 C       2.195367     1.797955    -2.147565      81.16
 H       1.543253     2.257726    -2.781350      26.65
 C       3.176560     1.497641     0.129776      46.13
 H       3.391580     1.704827     1.234283      20.67
 C       3.674410     0.274802    -0.397886      20.18
 O       4.355476    -0.608309     0.413628     262.44
 C       5.781624    -0.534392     0.724029     109.92
 H       6.419270    -1.149927     0.064044      27.34
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 H       5.817706    -1.154769     1.592275      27.73
 H       6.098885     0.538852     0.842488      27.92
 C       3.663662    -0.134948    -1.746486      20.33
 O       3.984846    -1.360985    -2.142990     146.03
 H       4.512359    -1.827414    -1.204107      18.24
 C       3.039312     0.726680    -2.642088      57.95
 H       3.115938     0.418486    -3.827039      20.05
 C       2.398767     2.322615    -0.749466      54.36
 C       1.820550     3.528686    -0.117457     103.57
 H       2.270942     4.364460    -0.423842      20.84
 O       2.162274     3.667398     1.389234     241.27
 H       2.859581     4.365763     1.169421      25.47
 C       0.177256     3.468207    -0.292181      75.93
 H      -0.311260     3.325688    -1.385843      20.72
 C      -0.207786     4.962953     0.226723      80.97
 O       0.480303     6.113826    -0.344318     235.56
 H       0.513457     5.912027    -1.299623      29.06
 H       0.093628     4.876732     1.346060      22.67
 H      -1.430122     5.249842     0.390095      22.44
 C      -1.318142    -0.830733    -0.194053      43.85
 H      -0.880174    -1.891194    -0.070942      20.12
 C      -3.325894     0.437536    -0.489563      58.27
 H      -4.244011     0.397356    -0.968921      17.54
 C      -2.480841     1.604247    -0.308169       0.96
 O      -2.892267     2.976361    -0.762213     122.61
 C      -4.400995     3.204123    -1.160264     106.99
 H      -5.069999     2.990536    -0.362425      27.83
 H      -4.199913     4.336443    -1.271870      24.58
 H      -4.591609     2.541761    -1.946227      26.68
 C      -1.150200     1.463100     0.060983      -0.06
 O      -0.413143     2.623234     0.758924     143.68
 C      -0.501605     0.203786     0.193493      50.85
 H       0.620389     0.162482     0.362331      20.97
 C      -2.629526    -0.753505    -0.642691      29.80
 C      -3.246752    -2.092008    -0.932721      84.13
 H      -4.080564    -1.796064    -1.510027      24.23
 O      -2.385495    -3.049657    -1.701183     231.88
 H      -2.812113    -4.030739    -1.695627      15.78
 C      -3.919202    -2.797353     0.272957      88.57
 H      -3.140515    -3.236420     0.976715      24.05
 O      -4.845095    -1.727267     0.847164     283.65
 H      -4.255434    -1.344639     1.680854      22.63
 C      -4.815830    -3.868321    -0.249307      81.76
 O      -4.264465    -4.971869    -0.952556     282.58
 H      -3.808355    -5.630770    -0.272073      27.73
 H      -5.618688    -3.458287    -0.952911      26.83
 H      -5.419576    -4.410262     0.807032      23.80
55
name = lig-etoh-frame_638
 C       2.217303     1.760545    -2.150014      59.73
 H       1.398711     2.358192    -2.761508      22.64
 C       3.126006     1.518575     0.093245      69.77
 H       3.450941     1.560301     1.105029      22.80
 C       3.634175     0.246873    -0.341534      30.18
 O       4.334191    -0.606895     0.416435     235.71
 C       5.819403    -0.610180     0.720327      90.97
 H       6.516237    -1.189913     0.106516      27.73
 H       5.917543    -1.087496     1.757799      26.96
 H       6.033732     0.582357     0.682840      26.74
 C       3.671329    -0.076826    -1.702799      28.39
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 O       4.006210    -1.366849    -2.128205     229.81
 H       4.419367    -1.909153    -1.615849      25.37
 C       2.937165     0.752122    -2.637637      54.45
 H       2.943363     0.443892    -3.578981      24.84
 C       2.447432     2.298644    -0.756643      51.59
 C       1.871118     3.501233    -0.152492      88.60
 H       2.300381     4.649753    -0.598016      17.45
 O       2.131352     3.652529     1.338358     256.60
 H       2.800891     4.425068     1.296313      24.70
 C       0.203287     3.498912    -0.281938      75.66
 H      -0.309077     3.339524    -1.132815      23.78
 C      -0.225924     5.015183     0.303770     106.67
 O       0.470612     6.078439    -0.361738     236.53
 H       0.425500     5.833961    -1.317984      28.43
 H       0.240543     5.080307     1.266013      23.19
 H      -1.242112     4.915067     0.122017      25.15
 C      -1.303969    -0.814995    -0.264591      50.20
 H      -0.894387    -1.758210    -0.071245      23.44
 C      -3.265297     0.501446    -0.559642      59.03
 H      -4.391586     0.443641    -0.838249      21.58
 C      -2.574982     1.648042    -0.267293     -15.80
 O      -2.928437     3.034065    -0.796598     130.66
 C      -4.318652     3.210033    -1.190694      95.54
 H      -4.779678     2.832105    -0.074884      24.38
 H      -4.217916     4.400756    -1.422141      23.45
 H      -4.666404     2.529470    -2.050775      24.89
 C      -1.072040     1.586007     0.097847     -23.06
 O      -0.407751     2.579366     0.666894     197.61
 C      -0.488197     0.255771     0.192885      34.74
 H       0.494441     0.097813     0.663800      22.16
 C      -2.619623    -0.802630    -0.666012      30.52
 C      -3.212565    -2.101723    -0.970670      85.67
 H      -4.081593    -2.024617    -1.781679      20.33
 O      -2.416184    -3.035013    -1.737747     224.71
 H      -3.144857    -3.806536    -1.842560      16.40
 C      -3.934399    -2.702227     0.282248      88.91
 H      -3.063066    -2.985674     0.885965      24.49
 O      -4.857161    -1.734671     0.858412     371.13
 H      -4.299281    -1.344257     1.500772      29.05
 C      -4.847905    -3.942907    -0.237815     109.76
 O      -4.257171    -5.073673    -0.919063     351.17
 H      -3.762902    -5.744642    -0.377903      29.32
 H      -5.557148    -3.502320    -0.903084      29.85
 H      -5.415130    -4.244469     0.494494      27.91
55
name = lig-etoh-frame_639
 C       2.200275     1.837756    -2.100567      53.80
 H       1.557318     2.345327    -2.740697      24.11
 C       3.141309     1.444870     0.085458      73.05
 H       3.340233     1.816986     1.125918      21.78
 C       3.634894     0.253025    -0.338664      24.78
 O       4.335852    -0.659346     0.473548     249.45
 C       5.826316    -0.647614     0.729561     114.92
 H       6.417786    -1.178229    -0.075478      27.70
 H       5.968268    -0.784618     1.820818      26.77
 H       6.169547     0.357436     0.653280      29.78
 C       3.640735    -0.043323    -1.675133      48.51
 O       4.011810    -1.345322    -2.160528     160.48
 H       4.641589    -2.097808    -1.606029      18.33
 C       2.867831     0.721926    -2.609613      66.71
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 H       2.633655     0.340906    -3.789293      22.06
 C       2.474753     2.259221    -0.810818      50.33
 C       1.856083     3.534051    -0.190181     111.17
 H       2.083574     4.322273    -0.735938      21.84
 O       2.100641     3.648427     1.253178     330.33
 H       2.789601     4.208417     1.563995      28.96
 C       0.275021     3.615027    -0.204804      62.66
 H      -0.168164     3.384046    -1.297990      20.06
 C      -0.207755     5.014249     0.353353      98.81
 O       0.455737     6.044830    -0.397409     217.13
 H       0.300820     5.953821    -1.447705      25.21
 H       0.067862     5.146657     1.403437      23.76
 H      -1.354610     4.818353    -0.013079      21.31
 C      -1.236315    -0.816793    -0.306293      32.27
 H      -0.726955    -1.911219    -0.180463      19.92
 C      -3.247448     0.517759    -0.669329      54.51
 H      -4.324505     0.688599    -0.647190      23.91
 C      -2.586051     1.757259    -0.266094     -17.06
 O      -2.937963     3.039659    -0.812282     191.27
 C      -4.229625     3.198155    -1.170355     131.32
 H      -4.815034     3.005699    -0.315278      28.82
 H      -4.513627     4.317357    -1.534957      25.05
 H      -4.661699     2.717118    -2.035993      27.33
 C      -1.064142     1.605502     0.136431       5.75
 O      -0.374129     2.580336     0.589320     194.22
 C      -0.526790     0.350125     0.173454      44.43
 H       0.314535     0.045747     0.954170      20.62
 C      -2.587305    -0.791061    -0.670408      20.93
 C      -3.280283    -2.109000    -1.071476      93.73
 H      -4.053640    -1.923331    -1.739562      22.99
 O      -2.447318    -3.035233    -1.751370     296.37
 H      -3.066049    -3.667066    -1.996901      22.32
 C      -3.950287    -2.641541     0.253026      84.43
 H      -3.127673    -2.828550     1.035838      20.46
 O      -4.862109    -1.767685     0.845299     307.35
 H      -4.393830    -1.160430     1.740650      21.12
 C      -4.859470    -3.998203    -0.217579      67.80
 O      -4.254852    -5.168404    -0.905423     317.13
 H      -3.603328    -5.640303    -0.360559      27.62
 H      -5.511141    -3.517590    -1.027534      26.99
 H      -5.699124    -4.300102     0.774423      24.39
55
name = lig-etoh-frame_640
 C       2.194396     1.918621    -2.084448      78.38
 H       1.591535     2.530610    -2.843051      23.05
 C       3.175546     1.392044     0.127208      31.58
 H       3.154652     1.999822     1.025192      22.74
 C       3.713270     0.232800    -0.329314      18.14
 O       4.353241    -0.718894     0.554432     246.58
 C       5.798193    -0.643236     0.724185     110.82
 H       6.192383    -1.322889    -0.012811      25.84
 H       6.015275    -0.840995     1.781222      26.06
 H       6.386610     0.436670     0.520089      24.67
 C       3.584973    -0.090140    -1.721460      17.40
 O       4.016647    -1.323748    -2.205633     159.96
 H       4.803741    -1.712144    -1.589242      18.69
 C       2.797046     0.660651    -2.603626      40.13
 H       2.516519     0.360122    -3.478486      23.96
 C       2.464121     2.255881    -0.816367      88.43
 C       1.801368     3.535889    -0.196906     102.87
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 H       2.142881     4.460016    -1.065142      19.48
 O       2.067160     3.648327     1.174150     266.42
 H       2.990871     3.955808     1.519404      27.93
 C       0.341648     3.714471    -0.163739      98.39
 H       0.210929     3.712884    -1.200308      21.46
 C      -0.214153     4.972777     0.336231     116.56
 O       0.437989     6.032525    -0.443695     269.49
 H       0.183538     5.997857    -1.342488      31.65
 H      -0.288081     5.139960     1.446653      25.38
 H      -1.244381     5.094589     0.257437      25.80
 C      -1.150761    -0.835566    -0.324325      49.86
 H      -0.663389    -1.704358    -0.360611      22.36
 C      -3.222978     0.553167    -0.746760      61.95
 H      -4.311390     0.694201    -0.746937      24.94
 C      -2.501621     1.817999    -0.315331       7.73
 O      -2.893822     3.028526    -0.804610     206.54
 C      -4.215367     3.223337    -1.164445     123.12
 H      -5.242578     3.120102    -0.423639      25.21
 H      -4.632184     4.257723    -1.507865      24.97
 H      -4.502117     2.573857    -2.072915      26.24
 C      -1.182330     1.591479     0.121144      16.89
 O      -0.296498     2.651587     0.570407     181.84
 C      -0.576538     0.355231     0.180049      49.72
 H       0.188732     0.261404     0.841245      23.01
 C      -2.550280    -0.742067    -0.694140       3.32
 C      -3.377271    -2.066673    -1.143953      64.09
 H      -4.290060    -1.605892    -1.771819      20.73
 O      -2.463471    -3.035575    -1.746646     225.22
 H      -2.978346    -3.920996    -2.258540      14.10
 C      -3.952699    -2.655482     0.223355      92.94
 H      -3.245579    -2.877317     0.986611      21.45
 O      -4.880362    -1.766203     0.846158     378.32
 H      -4.590260    -1.479236     1.625778      33.24
 C      -4.893343    -4.037677    -0.165899      94.80
 O      -4.268780    -5.241344    -0.879880     317.20
 H      -3.346692    -5.384571    -0.335697      23.97
 H      -5.441744    -3.684791    -1.012985      28.26
 H      -5.469378    -4.267404     0.591112      29.25
55
name = lig-etoh-frame_641
 C       2.209799     1.935404    -2.150963      23.37
 H       1.703335     2.693826    -2.786315      19.13
 C       3.175756     1.412902     0.140998      51.66
 H       3.189378     1.768881     1.187903      19.83
 C       3.823128     0.186148    -0.314504      35.28
 O       4.368707    -0.737310     0.622164     247.73
 C       5.786682    -0.610157     0.705152     118.93
 H       6.163018    -1.560236     0.158445      24.66
 H       6.092270    -1.081648     1.713000      26.39
 H       6.149604     0.278518     0.449955      29.43
 C       3.519586    -0.173049    -1.771856      19.35
 O       4.036882    -1.297932    -2.249561     174.99
 H       4.759202    -1.447465    -1.732169      21.09
 C       2.708216     0.664045    -2.541107      46.00
 H       2.402980     0.186112    -3.655485      21.83
 C       2.429697     2.270467    -0.748068      33.65
 C       1.811272     3.564418    -0.233114     125.81
 H       2.203947     4.331841    -0.732032      24.35
 O       2.077775     3.672056     1.147238     298.84
 H       3.095953     3.664087     1.052321      28.06
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 C       0.356617     3.750803    -0.184612      82.62
 H       0.160698     3.904032    -1.357923      17.98
 C      -0.239887     4.994286     0.318030     102.73
 O       0.424027     6.046239    -0.452953     226.59
 H       0.045174     5.935484    -1.425753      26.70
 H      -0.112425     5.140405     1.395539      25.46
 H      -1.414033     5.196297     0.232525      23.06
 C      -1.128874    -0.814554    -0.340852      44.95
 H      -0.442006    -1.810148    -0.497448      19.41
 C      -3.162585     0.600066    -0.774698      56.12
 H      -4.271824     0.498841    -1.081391      20.99
 C      -2.439360     1.784464    -0.426505      30.98
 O      -2.841565     3.054456    -0.769579     192.80
 C      -4.315486     3.233314    -1.193453     108.17
 H      -5.032801     2.989565    -0.489955      27.81
 H      -4.293000     4.400886    -1.520079      24.06
 H      -4.285452     2.463156    -1.951477      24.36
 C      -1.259794     1.645358     0.105978       8.11
 O      -0.242675     2.701665     0.578842     126.78
 C      -0.631308     0.309001     0.199211      19.14
 H       0.496741     0.529557     0.667368      20.14
 C      -2.526684    -0.691142    -0.753507       9.75
 C      -3.465474    -1.980020    -1.164129      70.56
 H      -4.247355    -1.635626    -1.748839      22.60
 O      -2.497385    -3.045524    -1.757429     278.97
 H      -2.873779    -3.794264    -2.140182      23.01
 C      -3.995275    -2.722610     0.172570      77.74
 H      -3.082607    -3.054039     0.832108      19.18
 O      -4.927543    -1.769691     0.806930     278.98
 H      -4.496303    -1.663645     1.902510      19.69
 C      -4.863941    -4.047593    -0.183162      71.61
 O      -4.269639    -5.280437    -0.815663     323.78
 H      -3.362770    -5.358919    -0.547097      29.30
 H      -5.644310    -3.732522    -0.958384      25.80
 H      -5.540584    -4.427200     0.900385      24.31
55
name = lig-etoh-frame_642
 C       2.250661     1.934828    -2.160055      31.23
 H       1.785276     2.672528    -2.796696      20.51
 C       3.178602     1.422796     0.134877      42.45
 H       3.314141     1.328688     1.240860      21.64
 C       3.861721     0.175285    -0.340469      10.63
 O       4.363950    -0.717371     0.666572     227.86
 C       5.794977    -0.691022     0.710924     103.96
 H       6.282596    -1.435661     0.108906      27.12
 H       6.111911    -0.917588     1.708971      27.37
 H       6.091308     0.482106     0.312966      23.55
 C       3.460106    -0.207597    -1.718586       1.45
 O       4.048671    -1.295903    -2.324736      94.48
 H       5.058863    -1.527533    -1.769549      18.89
 C       2.598331     0.665210    -2.539653      52.84
 H       2.499397     0.273860    -3.480085      25.39
 C       2.389811     2.263774    -0.716404      49.34
 C       1.832804     3.574939    -0.232837     107.41
 H       2.480253     4.621812    -0.639765      20.26
 O       2.154877     3.705137     1.153407     322.30
 H       3.088884     3.603566     1.028546      27.05
 C       0.286598     3.748520    -0.311516      74.51
 H      -0.173525     3.691270    -1.260851      23.45
 C      -0.280418     5.089896     0.318479     115.31
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 O       0.398907     6.082465    -0.457596     239.91
 H       0.147860     5.958276    -1.430208      27.70
 H       0.258888     5.182772     1.293533      24.56
 H      -1.296300     4.934958     0.119972      25.16
 C      -1.148718    -0.833937    -0.374542      36.49
 H      -0.562203    -1.647077    -0.491103      22.68
 C      -3.111556     0.583120    -0.811581      73.19
 H      -4.017250     0.539924    -1.312353      21.05
 C      -2.464594     1.768190    -0.579837      11.18
 O      -2.821542     3.106149    -0.721766     139.40
 C      -4.358543     3.244654    -1.249467      98.73
 H      -4.901739     2.840973    -0.220424      22.52
 H      -3.968197     4.279474    -1.536425      22.86
 H      -4.388244     2.526308    -2.087977      24.24
 C      -1.162757     1.675402     0.143722     -20.39
 O      -0.242408     2.699293     0.587501     140.78
 C      -0.613968     0.357397     0.247057      35.76
 H       0.382794     0.443094     0.269874      24.63
 C      -2.522127    -0.671156    -0.829639      23.79
 C      -3.471993    -1.924087    -1.123877      65.94
 H      -4.330892    -1.735498    -1.940881      21.49
 O      -2.532682    -3.009321    -1.759856     207.95
 H      -3.136445    -3.829172    -2.060549      18.72
 C      -4.050949    -2.794686     0.099355      82.34
 H      -3.137899    -3.060889     0.548947      23.99
 O      -4.949278    -1.791373     0.798143     337.91
 H      -4.570490    -1.707861     1.686077      26.94
 C      -4.866513    -4.072872    -0.186722     102.94
 O      -4.288551    -5.281363    -0.751872     379.17
 H      -3.302102    -5.517336    -0.554570      28.19
 H      -5.789690    -3.813727    -0.701216      27.22
 H      -5.181780    -4.341200     0.708905      28.58
55
name = lig-etoh-frame_643
 C       2.283790     1.940154    -2.089967      34.08
 H       1.796474     2.615435    -2.908517      20.28
 C       3.200360     1.367404     0.112014      41.43
 H       3.279598     1.298961     1.189269      21.72
 C       3.804328     0.201867    -0.397665      13.22
 O       4.349775    -0.677917     0.680299     199.12
 C       5.828326    -0.728739     0.707246     121.88
 H       6.368042    -1.331857    -0.089774      25.64
 H       6.139672    -0.630576     1.818552      25.37
 H       6.128609     0.163045     0.437979      29.50
 C       3.427024    -0.210978    -1.625009      13.77
 O       4.078912    -1.300898    -2.395562     182.49
 H       4.842302    -1.746016    -2.071533      25.83
 C       2.550280     0.626337    -2.520542      36.81
 H       2.486867     0.322485    -3.678729      23.11
 C       2.380313     2.245053    -0.723445      45.72
 C       1.867021     3.637702    -0.229038     103.55
 H       2.303686     4.363002    -0.738334      26.07
 O       2.233390     3.734666     1.181548     280.89
 H       3.289501     3.772959     1.381197      25.69
 C       0.196264     3.735595    -0.404915      51.89
 H      -0.381918     3.438658    -1.316650      22.71
 C      -0.246237     5.143983     0.285665     106.80
 O       0.365192     6.156159    -0.473378     254.70
 H       0.320439     6.066964    -1.432654      28.70
 H       0.234507     5.182273     1.272011      25.36
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 H      -1.394809     4.886778     0.297939      23.99
 C      -1.225172    -0.791377    -0.386916      28.06
 H      -0.601030    -1.804847    -0.459888      20.91
 C      -3.093971     0.561859    -0.884945      52.14
 H      -4.063342     0.743339    -1.539964      17.58
 C      -2.406708     1.808511    -0.654612      -4.77
 O      -2.843018     3.133181    -0.692521     140.91
 C      -4.310290     3.227777    -1.262121     111.15
 H      -4.861252     3.075722    -0.438929      28.00
 H      -4.297982     4.339864    -1.577737      25.82
 H      -4.669791     2.722697    -2.203484      24.48
 C      -1.052297     1.675191     0.158945      -2.09
 O      -0.277383     2.673949     0.592742     151.68
 C      -0.588427     0.407003     0.243871      44.77
 H       0.614852     0.218409     0.169917      22.93
 C      -2.510364    -0.731742    -0.878367      42.55
 C      -3.450839    -1.921948    -1.119426      96.26
 H      -4.158443    -1.749911    -1.871036      24.83
 O      -2.578886    -2.961706    -1.769022     211.91
 H      -3.360357    -3.693135    -1.866469      19.13
 C      -4.105496    -2.790399     0.001918      74.85
 H      -3.140578    -3.064064     0.611349      20.67
 O      -4.961979    -1.846894     0.768746     294.90
 H      -4.536556    -1.609611     1.766327      21.86
 C      -4.862918    -4.095516    -0.197334      74.12
 O      -4.311018    -5.271341    -0.720696     343.65
 H      -3.415610    -5.607322    -0.284477      25.61
 H      -5.880976    -3.936541    -0.631987      25.67
 H      -5.078280    -4.359783     1.116511      23.55
55
name = lig-etoh-frame_644
 C       2.281221     1.914679    -2.047980      45.46
 H       1.856689     2.538109    -2.748358      22.08
 C       3.186745     1.331855     0.080755      47.70
 H       3.180518     1.625127     1.152087      19.73
 C       3.733921     0.209997    -0.383252      18.92
 O       4.351979    -0.622334     0.658836     201.00
 C       5.852616    -0.734853     0.714670     101.22
 H       6.273693    -1.475092     0.024478      25.49
 H       6.154063    -0.792329     1.724594      26.74
 H       6.329333     0.409183     0.372913      23.90
 C       3.412596    -0.253602    -1.667383      17.47
 O       4.063444    -1.281745    -2.466192     156.07
 H       4.807676    -1.985578    -2.041473      20.95
 C       2.574182     0.564618    -2.487007      50.54
 H       2.470525     0.440686    -3.585941      25.22
 C       2.414575     2.243106    -0.706384      49.27
 C       1.880855     3.631701    -0.207311      77.56
 H       2.265603     4.444454    -1.147929      21.72
 O       2.288164     3.766755     1.225417     280.61
 H       3.199137     4.153540     1.319087      27.47
 C       0.143334     3.723247    -0.390332      59.72
 H      -0.224729     3.446292    -1.360714      23.92
 C      -0.217978     5.109955     0.211597     104.48
 O       0.330507     6.267647    -0.484853     238.12
 H       0.403651     6.099503    -1.541143      26.50
 H       0.081235     5.124123     1.266540      25.80
 H      -1.263709     5.324187     0.520119      25.59
 C      -1.262288    -0.742687    -0.361694      56.05
 H      -0.814421    -1.727271    -0.295299      22.29
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 C      -3.101219     0.612884    -1.008523      27.00
 H      -4.002810     0.778909    -1.464030      16.97
 C      -2.283090     1.820431    -0.635353      -3.16
 O      -2.906836     3.133641    -0.703641     190.82
 C      -4.209311     3.271261    -1.287389     125.77
 H      -5.139288     3.177383    -0.438278      23.98
 H      -4.796840     4.288500    -1.479665      24.19
 H      -4.678686     2.741025    -2.126497      24.91
 C      -1.028196     1.666131     0.102735      17.02
 O      -0.305516     2.682431     0.605172     180.99
 C      -0.507731     0.352238     0.167793      55.79
 H       0.475926     0.145542     0.482996      23.46
 C      -2.539173    -0.783538    -0.888980      22.12
 C      -3.400492    -1.964177    -1.157804      97.38
 H      -4.224637    -1.508000    -1.910988      21.77
 O      -2.640900    -2.926556    -1.781996     298.90
 H      -3.138157    -3.663505    -1.873477      25.60
 C      -4.103611    -2.715274    -0.028684      94.02
 H      -3.364320    -3.039974     0.655215      22.38
 O      -4.975454    -1.917898     0.745635     339.75
 H      -4.453058    -1.506110     1.606818      23.81
 C      -4.902238    -4.132467    -0.110304     104.77
 O      -4.321223    -5.271660    -0.712828     385.52
 H      -3.641838    -5.544371    -0.116879      31.21
 H      -5.882271    -4.080554    -0.607425      27.28
 H      -5.011783    -4.185270     0.834566      31.58
55
name = lig-etoh-frame_645
 C       2.260573     1.830972    -2.020730      44.29
 H       1.772974     2.646477    -2.734169      20.97
 C       3.117134     1.385167     0.097186      27.44
 H       3.272820     1.857149     1.076758      20.67
 C       3.699336     0.139601    -0.335992      23.31
 O       4.378442    -0.565434     0.623595     224.11
 C       5.863726    -0.666767     0.690379     108.43
 H       6.132480    -1.639762     0.196187      25.10
 H       6.130533    -1.119731     1.752708      25.09
 H       6.313524     0.150667     0.403606      29.32
 C       3.427083    -0.324267    -1.783126      21.72
 O       4.048028    -1.261494    -2.523272     163.45
 H       4.482274    -1.998197    -1.828440      22.61
 C       2.624234     0.555431    -2.445569      60.84
 H       2.478853     0.341213    -3.528561      24.52
 C       2.458996     2.264592    -0.689632      48.46
 C       1.886621     3.602730    -0.222076      97.10
 H       2.167039     4.308218    -0.835983      26.56
 O       2.293527     3.815204     1.240685     303.71
 H       3.152766     4.387869     1.049061      25.37
 C       0.169598     3.717141    -0.284402      76.35
 H       0.024574     3.587954    -1.381191      23.09
 C      -0.217686     5.090898     0.157889     100.50
 O       0.309827     6.372257    -0.504096     240.79
 H       0.330139     6.160156    -1.426678      30.86
 H       0.265098     5.049515     1.190270      25.18
 H      -1.224372     5.563726     0.326442      23.79
 C      -1.269399    -0.736354    -0.308125      45.24
 H      -0.840354    -1.760328    -0.094284      20.57
 C      -3.040588     0.664790    -1.111451      42.48
 H      -4.163502     0.807515    -1.431072      24.70
 C      -2.234208     1.787359    -0.605172       5.57
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 O      -2.957734     3.129925    -0.730470     185.57
 C      -4.230521     3.330251    -1.262909     128.94
 H      -4.917419     2.937228    -0.605484      28.89
 H      -4.470708     4.378070    -1.459986      26.70
 H      -4.303276     2.549398    -2.097998      24.71
 C      -1.035318     1.631853     0.006574      17.03
 O      -0.327507     2.724182     0.618491     202.30
 C      -0.457292     0.283528     0.071212      28.40
 H       0.457953     0.142087     0.821551      19.27
 C      -2.597426    -0.704602    -0.873908       6.11
 C      -3.418607    -1.980397    -1.234117     101.71
 H      -4.177762    -1.461727    -1.756699      22.59
 O      -2.657093    -2.918549    -1.831012     267.68
 H      -2.989664    -3.953042    -1.952290      16.82
 C      -4.092030    -2.653863    -0.004642      87.72
 H      -3.241977    -3.030720     0.699906      19.36
 O      -5.004361    -1.957995     0.733196     368.68
 H      -4.488785    -1.540363     1.393184      29.05
 C      -4.956671    -4.128523    -0.082945      62.17
 O      -4.326382    -5.274123    -0.715665     263.94
 H      -3.603540    -5.662366    -0.013535      23.59
 H      -5.940003    -4.027274    -0.565671      26.29
 H      -5.166306    -4.249161     1.240222      24.17
55
name = lig-etoh-frame_646
 C       2.207777     1.791584    -2.005063      57.72
 H       1.755356     2.410401    -2.678824      24.84
 C       3.085377     1.415237     0.157718      39.77
 H       3.485615     1.774671     1.109358      24.04
 C       3.655452     0.078180    -0.341548      18.57
 O       4.417893    -0.527464     0.608585     221.01
 C       5.839670    -0.683998     0.690467      99.68
 H       6.065105    -1.603843     0.065355      25.03
 H       5.975383    -1.007376     1.703504      26.54
 H       6.545178     0.278195     0.324548      24.69
 C       3.463216    -0.341604    -1.787995      17.39
 O       4.041252    -1.282733    -2.557801     238.72
 H       4.283761    -1.864067    -1.942323      29.31
 C       2.660694     0.582865    -2.467451      44.05
 H       2.418740     0.170272    -3.557823      22.10
 C       2.462422     2.298685    -0.727562      39.58
 C       1.844632     3.541279    -0.175035     101.73
 H       2.302716     4.632423    -0.724827      18.14
 O       2.269570     3.876193     1.212320     296.13
 H       3.192720     4.360493     1.052496      24.63
 C       0.272858     3.705828    -0.217952      83.25
 H       0.114678     3.578294    -1.318756      22.33
 C      -0.210360     5.152063     0.170205      95.64
 O       0.310850     6.441522    -0.510343     195.23
 H       0.262351     6.308428    -1.548274      25.77
 H       0.350610     5.200342     1.069723      24.28
 H      -1.345307     5.192520     0.074076      23.88
 C      -1.287235    -0.810836    -0.263817      20.70
 H      -0.919417    -1.843690     0.109589      20.03
 C      -2.984220     0.686974    -1.176751      71.73
 H      -4.011656     0.842859    -1.373996      27.34
 C      -2.329003     1.777657    -0.628439      -2.79
 O      -2.921605     3.118077    -0.722913     153.58
 C      -4.276177     3.321369    -1.266626     109.62
 H      -4.992121     2.697984    -0.524919      23.72
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 H      -3.942060     4.440167    -1.530659      22.03
 H      -4.069605     2.784548    -2.196198      24.86
 C      -0.983288     1.600881    -0.070659      -6.35
 O      -0.369684     2.749163     0.620079     188.68
 C      -0.420346     0.284655     0.013513      31.92
 H       0.265530     0.172930     0.880904      20.95
 C      -2.615540    -0.577110    -0.854213       8.66
 C      -3.490407    -1.947108    -1.256575      68.19
 H      -4.383924    -1.598185    -1.956228      21.60
 O      -2.620727    -2.956656    -1.930561     230.10
 H      -3.040715    -3.886634    -1.823361      18.86
 C      -4.063265    -2.691265     0.047242      94.42
 H      -3.138452    -2.888734     0.554770      22.75
 O      -5.059364    -1.959138     0.729369     300.90
 H      -4.500649    -1.308632     1.542159      21.26
 C      -4.991779    -4.103637    -0.021117      91.73
 O      -4.329223    -5.272668    -0.700055     349.54
 H      -3.601919    -5.704958    -0.247991      29.88
 H      -5.959847    -3.865719    -0.520425      27.46
 H      -5.243307    -4.385185     0.865869      29.21
55
name = lig-etoh-frame_647
 C       2.145820     1.778391    -2.008428      53.84
 H       1.525418     2.332928    -2.838838      22.99
 C       3.109490     1.377481     0.183748      52.22
 H       3.600011     1.569404     1.168352      23.89
 C       3.605458     0.086792    -0.384218      24.04
 O       4.442391    -0.504771     0.617632     229.87
 C       5.831141    -0.710989     0.652105     119.84
 H       6.150597    -1.436161    -0.073852      26.47
 H       5.978880    -0.789421     1.796418      25.07
 H       6.440871     0.111993     0.437051      28.06
 C       3.482725    -0.272293    -1.705522      20.56
 O       4.037506    -1.316439    -2.589910     165.60
 H       4.460145    -2.222867    -1.949720      20.72
 C       2.686922     0.579833    -2.537578      34.03
 H       2.393114     0.280622    -3.472146      24.13
 C       2.446272     2.303595    -0.735971      40.46
 C       1.827143     3.584617    -0.119022     122.22
 H       2.134134     4.336106    -0.651101      23.75
 O       2.240314     3.929447     1.180681     336.68
 H       3.184382     4.126276     1.247714      28.77
 C       0.405517     3.711283    -0.222767      69.20
 H       0.026990     3.460549    -1.220743      22.77
 C      -0.187922     5.229449     0.178100      89.26
 O       0.315193     6.468414    -0.520577     191.76
 H       0.212212     6.487532    -1.538618      26.00
 H       0.105710     5.556703     1.272107      23.02
 H      -1.225057     4.793126     0.123581      22.67
 C      -1.325650    -0.883244    -0.229728      42.43
 H      -1.103485    -1.841675     0.130687      22.02
 C      -2.981161     0.722353    -1.205426      71.04
 H      -4.038207     0.862290    -1.561985      27.20
 C      -2.398987     1.829622    -0.658662      -0.74
 O      -2.831111     3.078203    -0.679338     147.66
 C      -4.245981     3.278827    -1.289071     118.54
 H      -5.103154     3.016960    -0.741015      27.92
 H      -4.195335     4.304114    -1.367710      27.75
 H      -4.323678     3.058618    -2.416851      25.73
 C      -0.948070     1.611656    -0.139311     -11.39
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 O      -0.428685     2.740155     0.609090     149.51
 C      -0.443959     0.309426     0.000074      33.81
 H       0.374700     0.171781     0.742495      22.33
 C      -2.576964    -0.584217    -0.838574       6.64
 C      -3.575246    -1.900804    -1.266485      59.44
 H      -4.321010    -1.882225    -2.039363      21.88
 O      -2.592742    -2.977963    -2.014928     201.11
 H      -3.112056    -3.750165    -1.778190      20.71
 C      -4.059436    -2.765141     0.082724      81.38
 H      -3.069630    -2.833267     0.650081      20.55
 O      -5.093837    -1.906932     0.765375     349.31
 H      -4.797430    -1.425730     1.435352      31.36
 C      -4.956823    -4.070010    -0.026574      79.25
 O      -4.357075    -5.251989    -0.705406     310.38
 H      -3.506424    -5.621473    -0.288041      26.28
 H      -5.840721    -3.762097    -0.595586      26.19
 H      -5.355948    -4.548420     1.143778      23.10
55
name = lig-etoh-frame_648
 C       2.083104     1.778050    -2.062631      56.05
 H       1.375985     2.277160    -2.686942      22.72
 C       3.146321     1.322600     0.130675      51.97
 H       3.469803     1.490615     1.132819      23.36
 C       3.609933     0.147731    -0.364730      22.86
 O       4.423500    -0.491591     0.627352     205.01
 C       5.827561    -0.731905     0.626411     105.87
 H       6.313548    -1.517767    -0.073065      24.49
 H       6.151727    -0.869805     1.676308      26.11
 H       6.407754     0.364250     0.384282      23.69
 C       3.493564    -0.221218    -1.705465      42.93
 O       4.036620    -1.365543    -2.559397     214.13
 H       4.618768    -2.052935    -2.283521      24.00
 C       2.704404     0.596178    -2.553253      40.95
 H       2.363390     0.316081    -3.714804      21.79
 C       2.426966     2.257532    -0.670400      65.73
 C       1.875609     3.613377    -0.080044      97.58
 H       2.171971     4.468084    -1.096592      18.82
 O       2.206595     3.975643     1.190678     267.08
 H       3.275707     3.823065     1.333199      23.32
 C       0.446694     3.745797    -0.233297      51.64
 H       0.039919     3.505096    -1.257472      19.98
 C      -0.140745     5.285288     0.201873     103.95
 O       0.307004     6.470206    -0.525228     228.99
 H       0.178803     6.419251    -1.463227      29.48
 H      -0.274715     5.632245     1.179913      24.98
 H      -1.211897     4.906947     0.127041      23.05
 C      -1.366386    -0.872839    -0.213658      46.33
 H      -1.162980    -2.019248     0.139313      18.48
 C      -3.044852     0.735767    -1.204630      48.79
 H      -3.967582     0.782167    -1.858613      25.32
 C      -2.338431     1.841608    -0.675335       8.92
 O      -2.792547     3.068534    -0.647063     145.17
 C      -4.169602     3.276658    -1.345176     111.97
 H      -5.194747     3.079955    -0.780136      24.99
 H      -4.566812     4.448729    -1.091103      23.78
 H      -4.504518     3.090385    -2.350277      27.00
 C      -0.979451     1.654540    -0.188876       1.85
 O      -0.473065     2.717254     0.584449     128.71
 C      -0.519255     0.302382     0.029308      29.28
 H       0.633791     0.191677     0.346427      21.92
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 C      -2.565319    -0.683581    -0.856276       2.67
 C      -3.583162    -1.906984    -1.246303      54.19
 H      -4.376367    -1.802813    -2.045491      21.29
 O      -2.593641    -2.961061    -2.057475     145.23
 H      -3.189257    -3.903165    -1.864617      14.80
 C      -4.076483    -2.784796     0.124381      83.44
 H      -3.251141    -2.900441     0.817290      21.03
 O      -5.128523    -1.871065     0.771137     273.21
 H      -4.719843    -1.395256     1.723614      21.59
 C      -4.893953    -4.076538    -0.006668     108.70
 O      -4.389850    -5.218826    -0.723269     343.54
 H      -3.458500    -5.391151    -0.253352      27.25
 H      -5.728439    -3.770579    -0.666091      27.10
 H      -5.247531    -4.243960     0.897474      29.73
55
name = lig-etoh-frame_649
 C       2.057423     1.780683    -2.058991      46.90
 H       1.266436     2.363202    -2.594940      20.17
 C       3.149702     1.340318     0.069104      41.93
 H       3.264592     1.570636     1.165688      20.34
 C       3.703021     0.156146    -0.345055      21.40
 O       4.387392    -0.500871     0.640172     218.77
 C       5.871716    -0.694286     0.579701     110.86
 H       6.205266    -1.511684     0.028719      27.90
 H       6.223110    -1.078275     1.588964      26.79
 H       6.182669     0.260107     0.297519      28.05
 C       3.521813    -0.229247    -1.787285      10.73
 O       4.010547    -1.365260    -2.511505     104.57
 H       4.954086    -1.926019    -2.152175      19.69
 C       2.680623     0.635635    -2.582184      39.42
 H       2.586095     0.336314    -3.509565      26.12
 C       2.381913     2.185804    -0.628207      70.12
 C       1.963783     3.638001    -0.150129     108.38
 H       2.242855     4.260247    -0.856407      27.74
 O       2.205570     4.009037     1.235385     336.45
 H       3.127947     3.843660     1.286288      30.15
 C       0.383344     3.812061    -0.232995      52.50
 H       0.211726     3.749997    -1.298222      22.68
 C      -0.135404     5.296361     0.199330      99.22
 O       0.296292     6.456840    -0.515996     229.74
 H       0.165519     6.203853    -1.544889      25.87
 H      -0.245514     5.543974     1.330037      24.23
 H      -1.251641     5.322533    -0.132705      22.33
 C      -1.381514    -0.854053    -0.189628      38.88
 H      -1.056613    -1.770632     0.026812      20.62
 C      -3.093457     0.663627    -1.176314      44.42
 H      -3.854042     0.784915    -1.907617      17.40
 C      -2.254282     1.769942    -0.714367      10.41
 O      -2.829276     3.120688    -0.650041     145.03
 C      -4.157396     3.360557    -1.329198     117.31
 H      -4.765473     2.605268    -0.739856      24.72
 H      -4.336276     4.309421    -1.101784      28.32
 H      -4.229699     2.996986    -2.417176      24.80
 C      -1.033028     1.662388    -0.190985      10.97
 O      -0.480181     2.709368     0.544659     151.48
 C      -0.583146     0.285662     0.051917      41.71
 H       0.444311     0.196905     0.063497      24.30
 C      -2.645543    -0.744231    -0.921091       1.44
 C      -3.512267    -1.974868    -1.204663      72.99
 H      -4.382016    -1.491367    -1.760907      23.63
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 O      -2.650714    -2.940903    -2.047510     278.15
 H      -2.967094    -3.779401    -2.182262      25.00
 C      -4.110769    -2.725708     0.158282      80.49
 H      -3.323749    -2.941041     0.938122      21.27
 O      -5.137937    -1.830576     0.787791     297.18
 H      -4.607992    -1.719745     1.688368      22.97
 C      -4.850324    -4.051153    -0.062141      82.22
 O      -4.386567    -5.181260    -0.729544     347.86
 H      -3.561038    -5.435348    -0.385529      31.58
 H      -5.761623    -3.784118    -0.625445      27.53
 H      -5.318580    -4.185434     1.189410      25.48
55
name = lig-etoh-frame_650
 C       2.048194     1.799494    -1.993421      54.83
 H       1.332588     2.434901    -2.594280      18.63
 C       3.154896     1.379087     0.078962      39.43
 H       3.177579     1.651609     1.112889      18.46
 C       3.817715     0.125687    -0.411600      15.72
 O       4.369430    -0.550286     0.669713     207.87
 C       5.880117    -0.663505     0.549855      84.57
 H       6.025388    -1.548092    -0.236991      23.86
 H       6.184104    -1.055639     1.585727      25.33
 H       6.340203     0.364274     0.163440      24.50
 C       3.561322    -0.231237    -1.835741      14.34
 O       4.001229    -1.371675    -2.445213     100.05
 H       4.928331    -1.371126    -1.956797      20.60
 C       2.666377     0.671202    -2.567144      44.17
 H       2.672610     0.283913    -3.756758      22.91
 C       2.289415     2.156668    -0.682026      48.63
 C       1.959263     3.602303    -0.178250      82.93
 H       2.685068     4.515076    -0.861995      21.39
 O       2.204359     4.019428     1.266507     266.38
 H       3.288694     4.138185     1.381333      25.62
 C       0.306812     3.888759    -0.237052      65.58
 H       0.177832     3.933519    -1.376994      21.20
 C      -0.210397     5.276583     0.207699     110.54
 O       0.313325     6.434608    -0.525668     256.85
 H       0.286243     6.199551    -1.461603      30.87
 H       0.084310     5.326572     1.231524      26.39
 H      -1.230995     5.434883    -0.151952      23.96
 C      -1.427099    -0.802768    -0.200529      21.55
 H      -0.754975    -1.833650    -0.046324      18.25
 C      -3.093933     0.533679    -1.134829      59.42
 H      -3.946856     0.880764    -1.866366      17.29
 C      -2.300655     1.729985    -0.785566      -6.37
 O      -2.857799     3.163836    -0.678915     137.13
 C      -4.124434     3.351048    -1.285459     110.14
 H      -4.538278     2.400288    -0.847862      21.91
 H      -4.243729     4.590472    -1.157920      22.78
 H      -3.837807     3.153206    -2.327035      24.40
 C      -1.045213     1.619837    -0.134263       8.75
 O      -0.444825     2.735115     0.483115     153.15
 C      -0.654047     0.292449     0.049330      40.81
 H       0.564153     0.088792     0.112303      19.59
 C      -2.711705    -0.748780    -0.949212      29.80
 C      -3.442426    -2.051926    -1.147570      96.55
 H      -4.340466    -1.555995    -1.538091      24.30
 O      -2.713342    -2.885450    -2.016272     279.49
 H      -3.076237    -3.801033    -2.386069      21.54
 C      -4.127488    -2.642204     0.170751      88.93
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 H      -3.301135    -2.854526     0.873625      23.96
 O      -5.111162    -1.811323     0.801566     345.40
 H      -4.717907    -1.685319     1.695102      27.31
 C      -4.890206    -3.998421    -0.066705     105.45
 O      -4.366508    -5.151134    -0.746093     364.88
 H      -3.480114    -5.661228    -0.421381      25.33
 H      -5.861569    -3.772450    -0.538822      28.25
 H      -5.122951    -4.308257     0.829342      29.97
55
name = lig-etoh-frame_651
 C       2.030669     1.808548    -1.985314      45.16
 H       1.502441     2.436079    -2.641349      20.08
 C       3.176216     1.365248     0.078040      70.55
 H       3.311517     1.667463     1.144455      18.55
 C       3.859366     0.167602    -0.484277      52.42
 O       4.390651    -0.607158     0.686323     202.24
 C       5.851307    -0.657310     0.505241     118.34
 H       5.974096    -1.297602    -0.285140      28.53
 H       6.225931    -0.892610     1.471068      27.54
 H       6.479327     0.227983     0.223111      27.03
 C       3.557826    -0.170714    -1.826857      24.44
 O       4.017294    -1.363464    -2.369668     180.91
 H       4.857321    -1.390521    -2.016135      23.79
 C       2.686723     0.660796    -2.573573      19.95
 H       2.528492     0.546874    -3.560077      23.52
 C       2.224880     2.176986    -0.702656      58.06
 C       1.916211     3.627184    -0.173594     108.25
 H       2.550126     4.211136    -0.623149      29.85
 O       2.224445     3.994787     1.278912     283.63
 H       3.067254     4.520332     1.303609      29.11
 C       0.265898     3.936922    -0.310691      78.61
 H      -0.059885     3.863454    -1.326855      23.61
 C      -0.286110     5.252155     0.212369      99.74
 O       0.356487     6.404844    -0.529233     237.72
 H       0.415028     6.290592    -1.530211      28.86
 H       0.214366     5.322694     1.232844      25.54
 H      -1.455098     5.174747     0.242461      25.01
 C      -1.465553    -0.810918    -0.246740      53.34
 H      -0.928668    -1.647223    -0.222894      22.03
 C      -3.125681     0.511787    -1.140967      54.46
 H      -4.035328     0.678023    -1.589294      19.60
 C      -2.386509     1.734065    -0.816763     -10.85
 O      -2.820679     3.157678    -0.696763     178.25
 C      -4.050891     3.338732    -1.262599     131.71
 H      -4.989800     2.642604    -1.074010      24.46
 H      -4.493860     4.271506    -1.148920      28.40
 H      -3.878520     3.404648    -2.377606      26.11
 C      -1.086656     1.611257    -0.085877      -5.73
 O      -0.385562     2.776514     0.410632     162.10
 C      -0.633026     0.303692     0.049354      48.80
 H       0.262006     0.085824     0.419759      22.09
 C      -2.679821    -0.786954    -0.889201      37.73
 C      -3.461023    -2.070856    -1.090357      88.13
 H      -4.459601    -1.893328    -1.691052      21.88
 O      -2.748215    -2.852787    -1.995930     228.60
 H      -3.490736    -3.589857    -2.306034      20.10
 C      -4.099436    -2.605709     0.177728      92.45
 H      -3.251498    -2.782195     0.858992      23.13
 O      -5.073789    -1.792888     0.799656     298.14
 H      -4.856676    -1.359998     1.849217      23.05
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 C      -4.929648    -3.946235    -0.081023      82.61
 O      -4.329774    -5.134151    -0.795712     315.24
 H      -3.581280    -5.556051    -0.281599      26.56
 H      -5.912912    -3.744555    -0.554427      27.27
 H      -5.130618    -4.518642     1.087697      24.01
55
name = lig-etoh-frame_652
 C       2.024138     1.788606    -2.037118      84.94
 H       1.546188     2.511111    -2.836919      24.01
 C       3.183574     1.344811     0.046848      46.88
 H       3.538076     1.594505     1.050001      22.50
 C       3.824939     0.275717    -0.467214      37.68
 O       4.437879    -0.616038     0.652247     169.75
 C       5.817086    -0.655333     0.473289     113.49
 H       6.159242    -1.381163    -0.364224      25.72
 H       6.416051    -0.997937     1.468968      25.55
 H       6.343459     0.372179     0.260922      25.57
 C       3.545299    -0.115972    -1.800646      23.75
 O       4.024844    -1.343512    -2.305607      98.55
 H       5.099763    -1.822016    -2.100843      19.81
 C       2.696862     0.679007    -2.549768      30.35
 H       2.387737     0.602224    -3.709485      18.55
 C       2.235853     2.205746    -0.624666      72.23
 C       1.798885     3.643446    -0.112001      90.22
 H       2.619970     4.363312    -0.906056      20.18
 O       2.216206     3.949380     1.272119     283.48
 H       2.915084     4.596012     1.141782      27.45
 C       0.246016     3.929345    -0.418328      78.75
 H      -0.199508     3.744083    -1.453349      20.67
 C      -0.329879     5.237422     0.222878      98.87
 O       0.382960     6.359142    -0.520399     188.88
 H       0.390547     6.321156    -1.578976      26.14
 H       0.092789     5.450627     1.201814      24.78
 H      -1.343003     5.038002     0.630469      24.96
 C      -1.441787    -0.820968    -0.293970      49.11
 H      -0.985103    -1.959494    -0.243456      19.14
 C      -3.176943     0.576222    -1.154947      42.39
 H      -4.342040     0.458391    -1.393474      24.88
 C      -2.430148     1.746539    -0.774448       8.52
 O      -2.765455     3.094230    -0.702337     201.40
 C      -4.055122     3.333006    -1.321801     125.96
 H      -5.043628     2.856008    -1.199367      25.38
 H      -4.661022     4.342163    -0.850395      24.65
 H      -4.148437     3.511785    -2.400293      26.52
 C      -1.153912     1.652677    -0.087043      -8.09
 O      -0.334716     2.796031     0.352771     145.94
 C      -0.625085     0.318564     0.057318      29.24
 H       0.276408     0.111593     0.888202      18.85
 C      -2.661050    -0.806879    -0.813203      18.15
 C      -3.568248    -2.008269    -1.083123      87.72
 H      -4.404895    -1.901847    -1.733118      22.03
 O      -2.781357    -2.870573    -1.985592     286.71
 H      -3.444085    -3.413814    -2.155829      27.24
 C      -4.048713    -2.641166     0.224196      97.63
 H      -3.219464    -2.851375     0.961915      21.92
 O      -5.054022    -1.740241     0.808272     379.93
 H      -4.671168    -1.363784     1.510724      32.91
 C      -4.947681    -3.962581    -0.032534     101.55
 O      -4.304677    -5.091426    -0.854669     349.30
 H      -3.628129    -5.365477    -0.227597      29.28
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 H      -5.859556    -3.696708    -0.567458      28.92
 H      -5.201976    -4.242749     0.888042      29.63
55
name = lig-etoh-frame_653
 C       2.027265     1.819654    -2.045511      74.95
 H       1.563067     2.399368    -2.750944      24.87
 C       3.157386     1.409495     0.060012      35.46
 H       3.604006     1.619565     1.026351      23.10
 C       3.786397     0.313104    -0.423647      37.94
 O       4.463167    -0.583379     0.572953     204.89
 C       5.866130    -0.658148     0.451804     128.28
 H       6.255296    -1.324830    -0.297219      28.57
 H       6.293750    -1.085666     1.289256      29.08
 H       6.013983     0.450107     0.298452      25.25
 C       3.584041    -0.120850    -1.755245      15.15
 O       4.049617    -1.338588    -2.260482     199.02
 H       4.747658    -1.833345    -2.056739      26.02
 C       2.675491     0.715647    -2.578679      42.70
 H       2.533422     0.356441    -3.604889      22.59
 C       2.268916     2.221267    -0.586184      79.03
 C       1.731821     3.672969    -0.114950     108.15
 H       2.150664     4.294158    -0.766111      26.19
 O       2.174462     3.893741     1.241955     279.01
 H       2.963985     4.574645     1.086413      24.78
 C       0.210722     3.884451    -0.495133      84.96
 H       0.011713     3.826666    -1.557303      24.04
 C      -0.300781     5.217892     0.232560      98.14
 O       0.377293     6.315874    -0.512982     216.78
 H       0.204359     6.219119    -1.430193      31.27
 H       0.152674     5.401547     1.227631      24.79
 H      -1.439905     5.212755     0.439865      25.50
 C      -1.318263    -0.880914    -0.311509      44.77
 H      -1.077569    -1.872939    -0.061022      21.05
 C      -3.244543     0.608797    -1.134904      60.07
 H      -4.275918     0.600302    -1.231998      27.79
 C      -2.446788     1.739855    -0.696565      13.02
 O      -2.769448     3.029665    -0.738933     149.88
 C      -4.144277     3.422988    -1.379757     112.22
 H      -4.830243     2.447190    -1.063702      23.35
 H      -4.191746     4.197781    -0.676377      26.40
 H      -4.087302     3.611095    -2.470150      26.07
 C      -1.166431     1.669399    -0.114828       6.60
 O      -0.324406     2.769845     0.318361     158.61
 C      -0.625936     0.336798     0.112468      30.38
 H       0.073737     0.320748     0.832164      23.17
 C      -2.728658    -0.721731    -0.793593     -18.58
 C      -3.632274    -1.932528    -1.089173      58.68
 H      -4.581484    -1.485880    -1.672143      19.71
 O      -2.799548    -2.889287    -1.961489     159.26
 H      -3.439030    -3.797922    -2.214379      16.07
 C      -4.037677    -2.712923     0.269025      93.13
 H      -3.241336    -2.926723     0.967062      21.95
 O      -5.032479    -1.696741     0.794995     308.95
 H      -4.331765    -1.238162     1.557831      21.79
 C      -4.927245    -3.970616    -0.030783      74.68
 O      -4.302268    -5.015802    -0.889327     269.57
 H      -3.442848    -5.384842    -0.313715      22.99
 H      -5.803979    -3.590319    -0.616563      27.01
 H      -5.417838    -4.271514     1.164830      24.51
55
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name = lig-etoh-frame_654
 C       2.059250     1.860770    -1.990550      55.44
 H       1.342278     2.476912    -2.699792      18.93
 C       3.141995     1.518593     0.142404      36.39
 H       3.446982     1.838089     1.170700      21.32
 C       3.775646     0.256108    -0.396970      25.85
 O       4.442504    -0.543622     0.477594     244.79
 C       5.920935    -0.620433     0.418047     113.62
 H       6.276538    -1.188394    -0.474685      27.92
 H       6.192237    -1.138840     1.499605      25.08
 H       6.260487     0.427146     0.318719      28.50
 C       3.617098    -0.128750    -1.709909      12.33
 O       4.025165    -1.313277    -2.249443     130.19
 H       4.860146    -1.864108    -1.688600      18.99
 C       2.695060     0.702390    -2.581211      60.98
 H       2.620588     0.213479    -3.606445      25.32
 C       2.267170     2.266794    -0.647601      56.62
 C       1.686736     3.637345    -0.151172     107.26
 H       2.082892     4.685724    -0.886034      20.58
 O       2.122485     3.859541     1.199093     301.98
 H       2.979680     4.296206     1.248675      28.64
 C       0.176268     3.824839    -0.477045      76.97
 H       0.212445     3.919222    -1.617832      21.61
 C      -0.253192     5.196124     0.219382     104.75
 O       0.352319     6.278788    -0.492437     171.64
 H       0.024897     6.152217    -1.480832      27.23
 H       0.191004     5.085499     1.256234      24.64
 H      -1.290397     5.487534    -0.059878      24.08
 C      -1.262784    -0.875596    -0.317693      37.34
 H      -0.942009    -1.902034     0.142922      20.12
 C      -3.257764     0.613152    -1.054284      69.81
 H      -4.382575     0.881560    -1.256160      23.87
 C      -2.457173     1.715494    -0.629751      13.59
 O      -2.822848     3.011932    -0.815597     161.85
 C      -4.198866     3.453674    -1.378409     128.62
 H      -4.608080     2.563489    -1.142283      24.60
 H      -4.135158     4.373235    -0.663765      24.50
 H      -3.991046     3.726544    -2.433920      26.55
 C      -1.121149     1.631240    -0.145698      24.96
 O      -0.364595     2.706924     0.289407     173.65
 C      -0.677227     0.347694     0.154394      19.59
 H       0.330517     0.409751     0.848924      20.67
 C      -2.754342    -0.619054    -0.800360      -8.21
 C      -3.650485    -1.889031    -1.093045      67.63
 H      -4.480129    -1.423050    -1.433684      24.04
 O      -2.843796    -2.906006    -1.943257     217.77
 H      -3.155249    -3.832002    -2.025728      20.05
 C      -4.086424    -2.748273     0.257749      85.82
 H      -3.178676    -2.950030     0.932410      22.06
 O      -4.969145    -1.662427     0.807657     343.52
 H      -4.470074    -1.191141     1.595900      25.55
 C      -4.918424    -3.969865    -0.001807     110.52
 O      -4.292388    -4.938586    -0.885812     365.85
 H      -3.515699    -5.384050    -0.662141      31.22
 H      -5.716889    -3.575937    -0.614821      27.89
 H      -5.366875    -4.396643     0.783748      29.07
55
name = lig-etoh-frame_655
 C       2.090331     1.871826    -1.994949       8.50
 H       1.328622     2.394896    -2.477638      18.56
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 C       3.157891     1.580524     0.212016      49.82
 H       3.211217     1.986368     1.206983      18.89
 C       3.736625     0.274904    -0.350117      20.29
 O       4.440780    -0.530970     0.412163     227.49
 C       5.954418    -0.569814     0.411752     115.52
 H       6.267033    -1.043728    -0.571032      26.26
 H       6.130673    -1.023795     1.266228      29.50
 H       6.698940     0.347172     0.452666      27.45
 C       3.584399    -0.095718    -1.709902      17.24
 O       4.022795    -1.310383    -2.244757     174.98
 H       4.650597    -1.621088    -1.456319      20.38
 C       2.749000     0.674218    -2.521359      53.71
 H       2.534832     0.322553    -3.625035      24.89
 C       2.274577     2.337724    -0.719680      67.03
 C       1.699202     3.643451    -0.246267     123.08
 H       2.101553     4.457025    -0.695238      26.95
 O       2.051742     3.830521     1.171195     300.19
 H       3.026746     4.014826     1.270239      30.67
 C       0.177593     3.770835    -0.412160      93.42
 H       0.074758     3.797448    -1.497345      23.77
 C      -0.225062     5.146758     0.163753     117.45
 O       0.348209     6.260544    -0.485499     259.04
 H       0.094236     6.248745    -1.447286      29.68
 H      -0.031963     4.992855     1.208064      27.49
 H      -1.280501     5.354409    -0.041929      25.64
 C      -1.308486    -0.806131    -0.304195      42.94
 H      -0.911988    -1.778366     0.112074      21.22
 C      -3.271034     0.654840    -0.939191      59.18
 H      -4.230363     0.907094    -1.388674      23.54
 C      -2.460537     1.718459    -0.596606      15.70
 O      -2.876118     3.033702    -0.903137     205.89
 C      -4.149411     3.497310    -1.335500     116.39
 H      -5.136039     2.621076    -1.261760      23.17
 H      -4.630950     4.452046    -0.889173      25.64
 H      -4.076509     3.776186    -2.393254      26.72
 C      -1.102791     1.579402    -0.181787      20.63
 O      -0.429920     2.642799     0.266886     219.24
 C      -0.674705     0.319445     0.212534      42.56
 H       0.346981     0.297458     0.504411      23.08
 C      -2.698387    -0.641800    -0.801470      11.43
 C      -3.596275    -1.919715    -1.057919      66.99
 H      -4.671766    -1.571545    -1.539955      22.05
 O      -2.872366    -2.873284    -1.932884     227.35
 H      -3.275811    -3.777466    -1.718014      16.86
 C      -4.112584    -2.689011     0.237901      97.30
 H      -3.244006    -2.912605     0.800473      24.61
 O      -4.911011    -1.645191     0.833204     371.94
 H      -4.569772    -1.319707     1.718778      28.27
 C      -4.908349    -3.957143    -0.029515      84.64
 O      -4.293568    -4.874484    -0.905668     308.33
 H      -3.453513    -5.414547    -0.610206      25.44
 H      -5.798430    -3.618974    -0.647623      25.28
 H      -5.408554    -4.686102     0.934354      24.24
55
name = lig-etoh-frame_656
 C       2.131728     1.839556    -2.033492      17.91
 H       1.309358     2.334572    -2.647612      19.62
 C       3.159051     1.598255     0.191115      70.49
 H       3.130814     1.913638     1.266524      19.03
 C       3.663134     0.409399    -0.305548      30.42
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 O       4.489618    -0.545391     0.400248     216.30
 C       5.989510    -0.495179     0.372534     110.48
 H       6.295152    -1.004598    -0.491867      28.19
 H       6.236529    -1.311534     1.305479      25.30
 H       6.562993     0.369275     0.584562      29.13
 C       3.519130    -0.058974    -1.720990      20.46
 O       4.022190    -1.288659    -2.214740     188.96
 H       4.495963    -1.648089    -1.518830      24.70
 C       2.757058     0.697502    -2.480583      43.30
 H       2.493557     0.477119    -3.459906      25.78
 C       2.347332     2.368630    -0.732091      68.52
 C       1.718902     3.629324    -0.295981     107.63
 H       2.391278     4.600988    -0.887285      18.09
 O       1.976688     3.808803     1.158288     259.25
 H       3.017661     3.790369     1.168317      27.69
 C       0.201548     3.713216    -0.374333      94.60
 H      -0.237993     3.586491    -1.421538      21.05
 C      -0.267189     5.072159     0.099632     100.49
 O       0.374303     6.260226    -0.479411     254.78
 H       0.249372     6.292191    -1.442175      30.34
 H      -0.187617     5.246137     1.258669      24.92
 H      -1.420305     4.929451     0.204805      24.23
 C      -1.422848    -0.744816    -0.269300      52.01
 H      -1.032495    -1.756359    -0.126535      20.87
 C      -3.261102     0.660030    -0.831469      40.79
 H      -4.185472     0.754042    -1.439949      19.61
 C      -2.476878     1.762497    -0.600477      14.80
 O      -2.912692     3.080967    -0.970561     245.93
 C      -4.175113     3.505376    -1.322316     143.03
 H      -5.119769     3.024802    -1.350628      26.87
 H      -4.767313     4.382920    -0.865832      26.23
 H      -4.173923     3.739207    -2.409836      27.30
 C      -1.136568     1.542675    -0.206468      13.43
 O      -0.474865     2.621156     0.275576     219.52
 C      -0.638280     0.286825     0.218714      49.59
 H       0.477688     0.123072     0.398454      22.01
 C      -2.645332    -0.718139    -0.792130      26.99
 C      -3.552392    -1.957040    -1.045733      98.64
 H      -4.372648    -1.803450    -1.624971      23.58
 O      -2.891267    -2.831795    -1.928902     277.15
 H      -3.456852    -3.645197    -1.467226      14.38
 C      -4.105505    -2.581225     0.230442      82.69
 H      -3.179345    -2.918225     0.859987      21.32
 O      -4.874618    -1.627832     0.856858     313.89
 H      -4.573689    -1.681206     1.973539      21.53
 C      -4.963573    -3.963409    -0.043592     101.79
 O      -4.263517    -4.846870    -0.957994     332.39
 H      -3.614180    -5.303865    -0.289276      25.93
 H      -5.893246    -3.719764    -0.518821      28.49
 H      -5.128255    -4.422882     0.854154      30.28
55
name = lig-etoh-frame_657
 C       2.143420     1.864368    -2.042205      73.95
 H       1.534769     2.264190    -2.876848      25.07
 C       3.133544     1.622891     0.152418      62.36
 H       3.235945     1.714038     1.209804      21.24
 C       3.656352     0.476306    -0.314050      32.13
 O       4.541658    -0.544896     0.414442     203.30
 C       6.005440    -0.482187     0.384184     108.69
 H       6.455280    -0.878718    -0.639821      25.75
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 H       6.301044    -1.230113     0.977249      28.21
 H       6.235254     0.647301     0.713788      25.05
 C       3.492772    -0.057852    -1.649336      24.44
 O       4.002725    -1.228521    -2.184603     124.44
 H       4.533715    -1.937370    -1.423352      21.02
 C       2.712806     0.750850    -2.509573      47.96
 H       2.445790     0.391181    -3.672851      18.54
 C       2.432384     2.356285    -0.751846      59.91
 C       1.770633     3.648346    -0.316050     119.77
 H       2.176548     4.391184    -0.885933      21.06
 O       1.923825     3.791427     1.135866     341.94
 H       2.855651     3.809000     1.237696      28.96
 C       0.208722     3.654295    -0.417122      84.39
 H      -0.264300     3.547840    -1.398135      22.30
 C      -0.361852     5.019526     0.108867      94.09
 O       0.380530     6.244392    -0.470514     187.07
 H       0.390119     6.211495    -1.542241      26.09
 H      -0.050931     5.345614     1.047233      24.31
 H      -1.411764     4.812894     0.036498      25.24
 C      -1.477450    -0.778232    -0.193696      37.90
 H      -1.043405    -1.870375    -0.438197      19.12
 C      -3.250191     0.594005    -0.772103      47.95
 H      -4.264105     0.598675    -1.334416      16.05
 C      -2.526099     1.807695    -0.635664      11.67
 O      -2.912971     3.122354    -1.003213     196.56
 C      -4.261829     3.546177    -1.370449     103.87
 H      -5.208066     2.650506    -1.255901      22.07
 H      -4.313434     4.453470    -0.591317      23.89
 H      -4.177265     3.827619    -2.433625      25.92
 C      -1.161375     1.541056    -0.184348      10.34
 O      -0.485166     2.636280     0.336996     221.05
 C      -0.606009     0.282832     0.160946      43.37
 H       0.484561     0.033358     0.433109      19.94
 C      -2.712203    -0.714542    -0.780858      34.09
 C      -3.500823    -1.938708    -1.054987      79.00
 H      -4.452510    -1.539905    -1.744188      21.63
 O      -2.891640    -2.838856    -1.914660     287.90
 H      -3.202237    -3.744390    -1.828255      20.46
 C      -4.065417    -2.535622     0.233138      90.11
 H      -3.283464    -2.878765     0.859479      24.18
 O      -4.862834    -1.613369     0.913501     384.52
 H      -4.598668    -1.617537     1.747878      32.32
 C      -5.004530    -3.907500    -0.075753      65.35
 O      -4.222031    -4.839222    -0.986648     324.70
 H      -3.719882    -5.295733    -0.362213      28.70
 H      -6.084285    -3.744830    -0.400005      26.83
 H      -5.029125    -4.357322     1.132518      26.09
55
name = lig-etoh-frame_658
 C       2.145216     1.937052    -2.071307      82.45
 H       1.675459     2.543197    -2.837305      27.45
 C       3.129550     1.624317     0.149408      55.56
 H       3.349798     1.786795     1.226021      22.17
 C       3.752527     0.396638    -0.367416      36.30
 O       4.560092    -0.530372     0.439338     251.85
 C       5.998651    -0.423819     0.356658     110.26
 H       6.447719    -0.386239    -0.613715      27.55
 H       6.485724    -1.291272     1.103681      24.54
 H       6.148445     0.520357     0.718320      27.91
 C       3.465020    -0.049394    -1.580797      19.07
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 O       3.988782    -1.181921    -2.140182     251.79
 H       4.402990    -1.772108    -1.543750      27.80
 C       2.682478     0.721347    -2.592529      12.39
 H       2.537743     0.367942    -3.489426      19.92
 C       2.455019     2.386661    -0.790529      48.30
 C       1.776785     3.616782    -0.288656     109.27
 H       2.037902     4.665752    -1.045067      17.79
 O       1.888736     3.788242     1.108326     308.57
 H       2.833419     4.002633     1.428803      26.02
 C       0.193193     3.622492    -0.485409      73.99
 H      -0.019349     3.582708    -1.592345      21.17
 C      -0.414071     4.989468     0.108670      82.70
 O       0.359916     6.208909    -0.490929     196.70
 H       0.382239     6.080881    -1.426491      31.17
 H       0.024282     5.107821     1.186752      22.36
 H      -1.514596     5.082781    -0.252094      23.53
 C      -1.448222    -0.892614    -0.142561      41.47
 H      -0.989286    -1.780818    -0.359574      20.48
 C      -3.298156     0.556780    -0.783164      64.43
 H      -4.316081     0.595157    -1.077558      19.06
 C      -2.561636     1.798905    -0.676530       2.43
 O      -2.892858     3.132426    -1.020486     163.69
 C      -4.350132     3.564970    -1.388117     119.08
 H      -4.899906     2.684257    -1.156513      24.64
 H      -4.203688     4.372288    -0.669376      25.53
 H      -4.311358     3.989679    -2.408506      26.64
 C      -1.178640     1.589596    -0.125246       4.62
 O      -0.470887     2.663192     0.426997     204.93
 C      -0.623371     0.268269     0.061147      29.39
 H       0.354157     0.168649     0.466373      19.63
 C      -2.777278    -0.663597    -0.729244      21.33
 C      -3.541843    -1.884780    -1.109645      80.75
 H      -4.342469    -1.360855    -1.468829      24.74
 O      -2.839153    -2.861459    -1.923372     270.11
 H      -3.056639    -3.844764    -2.130139      18.79
 C      -4.064743    -2.549067     0.212766      76.96
 H      -3.203693    -2.919928     0.895697      21.14
 O      -4.888424    -1.597047     0.923274     300.69
 H      -4.402214    -1.284237     2.037273      18.38
 C      -5.000765    -3.833931    -0.058912      89.50
 O      -4.214356    -4.825582    -0.997134     296.21
 H      -3.577743    -5.524886    -0.475035      24.74
 H      -6.025717    -3.727342    -0.358104      28.49
 H      -5.029756    -4.288363     0.882395      29.44
55
name = lig-etoh-frame_659
 C       2.174274     1.984585    -2.167660      64.97
 H       1.737881     2.937574    -2.676572      21.29
 C       3.185746     1.555585     0.141871      46.03
 H       3.366078     2.047413     1.113013      24.71
 C       3.865714     0.334543    -0.337922      41.94
 O       4.552470    -0.519122     0.462400     263.15
 C       5.995651    -0.361890     0.352881     103.32
 H       6.352124    -0.067007    -0.705143      25.60
 H       6.508892    -1.065714     0.920098      26.87
 H       6.365244     0.641001     0.969595      25.25
 C       3.408953    -0.042867    -1.638490      26.56
 O       3.970562    -1.149617    -2.123570     209.45
 H       4.442492    -1.687217    -1.395940      23.70
 C       2.667014     0.707340    -2.569132      27.10
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 H       2.561336     0.191955    -3.725728      18.59
 C       2.448425     2.431604    -0.798608      39.15
 C       1.733521     3.632341    -0.286966     118.34
 H       1.991705     4.512692    -0.764414      22.59
 O       1.881217     3.799847     1.106258     300.63
 H       2.726443     4.302710     1.410170      26.45
 C       0.169303     3.634883    -0.530400      60.28
 H       0.145839     3.447355    -1.633055      18.71
 C      -0.406127     4.987987     0.067089     100.05
 O       0.323561     6.158010    -0.494882     222.64
 H       0.273327     5.985981    -1.523607      28.09
 H      -0.362107     4.730175     1.098937      26.05
 H      -1.377514     5.315303    -0.180653      25.79
 C      -1.422794    -0.945370    -0.146508      44.67
 H      -0.828260    -2.031582    -0.124599      18.34
 C      -3.379012     0.625884    -0.833853      48.80
 H      -4.567884     0.689128    -0.881961      19.52
 C      -2.545494     1.762352    -0.695698       3.33
 O      -2.871244     3.115487    -1.042902     130.18
 C      -4.346024     3.585777    -1.390391      93.00
 H      -5.006685     2.556543    -0.992222      21.64
 H      -4.632094     4.525161    -0.605024      24.63
 H      -4.531883     3.976965    -2.404540      25.94
 C      -1.223950     1.634727    -0.066063       3.09
 O      -0.449807     2.684577     0.493522     180.06
 C      -0.693749     0.260384    -0.037065      18.50
 H       0.362622     0.382661     0.542891      18.16
 C      -2.727746    -0.692201    -0.632947      12.15
 C      -3.612003    -1.867142    -1.126439      58.23
 H      -4.622869    -1.436462    -1.620195      22.09
 O      -2.742246    -2.852758    -1.964303     180.70
 H      -3.388416    -3.657288    -1.956125      17.30
 C      -4.088584    -2.584444     0.198555      95.01
 H      -3.213762    -2.896168     0.712705      23.88
 O      -4.903781    -1.566100     0.965933     386.64
 H      -4.443497    -1.274419     1.657616      33.67
 C      -4.923122    -3.780353    -0.054829      79.81
 O      -4.230361    -4.817608    -0.993191     281.76
 H      -3.603347    -5.459708    -0.595340      27.03
 H      -5.927089    -3.583809    -0.547179      25.99
 H      -5.100689    -4.432913     1.023241      24.98
55
name = lig-etoh-frame_660
 C       2.231930     2.057247    -2.222797      32.56
 H       1.821489     2.808168    -2.809346      19.45
 C       3.258729     1.506951     0.097481      41.78
 H       3.406976     2.089956     0.998135      24.16
 C       3.875551     0.372120    -0.306548      49.12
 O       4.569029    -0.522823     0.493633     269.42
 C       6.011065    -0.209889     0.362967     107.73
 H       6.193767    -0.074042    -0.673722      28.24
 H       6.607100    -1.242722     0.726431      24.56
 H       6.337128     0.475217     1.020745      28.05
 C       3.381590    -0.031966    -1.694934      23.25
 O       3.961453    -1.174739    -2.140400     152.77
 H       4.534004    -1.524079    -1.200001      18.68
 C       2.631388     0.722324    -2.574096      30.27
 H       2.570055     0.326516    -3.459186      24.25
 C       2.456009     2.392110    -0.808762      79.06
 C       1.660366     3.645026    -0.270340     103.24
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 H       2.229086     4.722859    -0.728648      19.05
 O       1.890524     3.828657     1.148053     305.11
 H       2.566426     4.468612     1.157760      29.26
 C       0.152668     3.664723    -0.533734      72.79
 H      -0.088857     3.247435    -1.522954      21.53
 C      -0.387754     4.986827    -0.021535     102.56
 O       0.300273     6.104316    -0.492507     252.53
 H       0.144756     6.047057    -1.499745      29.11
 H      -0.585000     4.706355     1.085659      24.17
 H      -1.532967     5.201308    -0.135733      23.45
 C      -1.388424    -0.965202    -0.189257      55.78
 H      -1.069319    -1.867445     0.025510      20.42
 C      -3.423822     0.680631    -0.865739      40.22
 H      -4.425981     0.747046    -0.881617      23.09
 C      -2.532253     1.765964    -0.696736       5.00
 O      -2.876333     3.108375    -1.075966     170.31
 C      -4.334277     3.567531    -1.318132     124.09
 H      -5.066282     2.866333    -1.125570      27.95
 H      -4.808282     4.373656    -0.721772      27.49
 H      -4.534872     3.752255    -2.377193      27.46
 C      -1.277701     1.624389    -0.032242       8.18
 O      -0.441848     2.681740     0.510290     173.78
 C      -0.730449     0.316606    -0.058929      37.60
 H       0.183529     0.330161     0.347742      19.81
 C      -2.723692    -0.737084    -0.574818      -7.56
 C      -3.669593    -1.860847    -1.114946      71.64
 H      -4.432339    -1.788346    -1.851207      21.45
 O      -2.684691    -2.817428    -1.991639     194.26
 H      -3.406365    -3.434509    -1.809490      20.36
 C      -4.113255    -2.575987     0.182901      86.21
 H      -3.115804    -2.845814     0.687361      21.71
 O      -4.938127    -1.572536     0.939511     293.05
 H      -4.192308    -1.231856     1.852573      18.05
 C      -4.858574    -3.818036    -0.034369     103.63
 O      -4.270195    -4.791672    -0.992962     311.99
 H      -3.586460    -5.294929    -0.486753      28.02
 H      -5.661004    -3.445786    -0.667431      27.20
 H      -5.285209    -4.302779     0.836478      27.61
55
name = lig-etoh-frame_661
 C       2.310603     2.106681    -2.198255      21.83
 H       1.799568     2.616218    -3.144510      16.34
 C       3.287937     1.571589     0.048805      42.55
 H       3.512992     1.913827     1.094002      19.09
 C       3.801532     0.403998    -0.356162       4.63
 O       4.607156    -0.516695     0.521020     242.83
 C       6.038724    -0.142792     0.387008      99.78
 H       6.196805     0.079743    -0.721075      27.68
 H       6.474042    -1.114060     0.316536      26.66
 H       6.336632     0.687420     1.187085      25.46
 C       3.413326    -0.025547    -1.684359      15.53
 O       3.967784    -1.231253    -2.144156     235.99
 H       4.433123    -1.473390    -1.475286      27.30
 C       2.601824     0.784820    -2.560666      72.45
 H       2.449111     0.340777    -3.724928      23.75
 C       2.453253     2.331551    -0.841456      72.60
 C       1.660185     3.670315    -0.269452     111.53
 H       2.091015     4.454785    -0.758023      27.50
 O       1.901745     3.860841     1.199842     283.08
 H       2.533393     4.644340     1.070580      26.88
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 C       0.128802     3.661228    -0.507782      69.89
 H      -0.388102     3.221130    -1.407405      22.41
 C      -0.464396     4.967185    -0.085001     110.01
 O       0.290542     6.079267    -0.495056     291.69
 H       0.146491     6.174509    -1.437614      32.44
 H      -0.305744     5.100919     0.999769      26.02
 H      -1.493675     4.842611    -0.380646      26.29
 C      -1.416289    -0.881084    -0.259015      34.17
 H      -1.089142    -2.004813     0.116647      17.64
 C      -3.345446     0.657467    -0.857518      41.30
 H      -4.531858     0.779266    -1.072853      20.77
 C      -2.572890     1.815056    -0.688997      16.92
 O      -2.914425     3.116660    -1.101909     210.90
 C      -4.295116     3.508839    -1.256114     105.06
 H      -5.300418     2.692199    -1.160861      22.93
 H      -4.638048     4.574850    -0.673144      24.41
 H      -4.267635     3.618996    -2.387089      25.11
 C      -1.300887     1.608095    -0.026676      19.40
 O      -0.456631     2.652914     0.492329     194.08
 C      -0.750259     0.360314    -0.025075      39.93
 H       0.437148     0.198187     0.242089      16.77
 C      -2.819652    -0.718572    -0.599071      17.28
 C      -3.638767    -1.874205    -1.088462      67.75
 H      -4.351310    -1.753347    -1.974808      19.50
 O      -2.660119    -2.757894    -1.989267     144.62
 H      -3.132357    -3.778019    -1.957268      16.58
 C      -4.090081    -2.539733     0.196229      97.08
 H      -3.176889    -2.691316     0.755538      23.15
 O      -4.932208    -1.594613     0.915806     391.94
 H      -4.612533    -1.437100     1.728599      30.68
 C      -4.861363    -3.865718    -0.073865      84.65
 O      -4.303359    -4.770803    -0.976584     279.26
 H      -3.468067    -5.164699    -0.423743      24.94
 H      -5.695105    -3.414408    -0.674427      25.81
 H      -5.447707    -4.324146     0.937960      25.13
55
name = lig-etoh-frame_662
 C       2.360996     2.104044    -2.208744      34.89
 H       1.808180     2.593722    -2.949531      18.89
 C       3.283151     1.694202     0.032113      51.58
 H       3.476266     1.801381     1.075149      19.60
 C       3.734354     0.368289    -0.428407      -1.46
 O       4.630043    -0.471555     0.517853     251.81
 C       6.043336    -0.088367     0.370714     106.58
 H       6.234831     0.534665    -0.519069      29.95
 H       6.638960    -1.095584     0.344850      25.85
 H       6.371320     0.612225     1.100797      29.02
 C       3.458398    -0.038034    -1.685093      14.83
 O       3.944174    -1.271476    -2.172922     170.99
 H       4.669268    -1.744309    -1.406241      19.23
 C       2.629719     0.799466    -2.578846      58.26
 H       2.347605     0.554413    -3.546369      25.57
 C       2.427430     2.366217    -0.821476      64.51
 C       1.681479     3.613149    -0.258615      88.62
 H       2.045549     4.565222    -1.080031      20.60
 O       1.919091     3.907602     1.213465     275.23
 H       2.555153     4.697836     1.341412      27.63
 C       0.094345     3.600496    -0.455702      82.35
 H      -0.254198     3.423889    -1.476267      21.08
 C      -0.548999     4.945273    -0.100633      98.93
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 O       0.282288     6.091292    -0.522232     213.56
 H       0.231910     6.296047    -1.570468      28.99
 H      -0.264871     5.236304     0.923438      23.37
 H      -1.560513     4.805447    -0.579527      23.69
 C      -1.509280    -0.780739    -0.310767      48.10
 H      -1.041477    -1.684856    -0.126958      19.84
 C      -3.291199     0.605860    -0.849101      60.42
 H      -4.194008     0.710452    -1.322612      23.71
 C      -2.604479     1.853191    -0.651730      21.02
 O      -2.956685     3.111859    -1.095170     260.95
 C      -4.297233     3.447302    -1.246625     132.23
 H      -4.939192     2.712548    -1.003544      28.42
 H      -4.290736     4.444063    -0.712986      25.70
 H      -4.247599     3.742200    -2.289592      26.51
 C      -1.300789     1.647987    -0.046225      19.78
 O      -0.486654     2.614937     0.467734     230.31
 C      -0.704032     0.322145     0.038706      30.17
 H       0.292259     0.276765     0.150434      19.97
 C      -2.890774    -0.636537    -0.677229      31.58
 C      -3.569183    -1.911961    -1.105173      67.41
 H      -4.430307    -1.451423    -1.686655      21.14
 O      -2.650507    -2.725255    -1.965761     275.31
 H      -2.730453    -3.593102    -2.084677      23.83
 C      -4.068207    -2.531788     0.231924      94.44
 H      -3.167511    -2.654953     0.910589      20.31
 O      -4.951405    -1.634848     0.842472     297.41
 H      -4.765479    -1.529309     1.987037      21.37
 C      -4.948455    -3.856947    -0.103872      89.23
 O      -4.292450    -4.784658    -0.948300     361.35
 H      -3.542517    -5.174811    -0.597500      31.17
 H      -5.882129    -3.510587    -0.578463      27.15
 H      -5.285488    -4.312161     0.856212      26.73
55
name = lig-etoh-frame_663
 C       2.372602     2.066683    -2.199910      22.60
 H       1.721352     2.853324    -2.770548      16.26
 C       3.283586     1.723635     0.014568      42.90
 H       3.340349     1.963546     1.120584      17.76
 C       3.710244     0.370360    -0.420416      11.02
 O       4.628349    -0.398332     0.476351     259.38
 C       6.040679    -0.042802     0.327780     107.41
 H       6.217591     0.758207    -0.399729      30.32
 H       6.827690    -0.851490     0.459420      26.15
 H       6.412888     0.520769     1.320421      27.14
 C       3.490819    -0.092069    -1.745588      12.48
 O       3.921019    -1.312296    -2.191369     205.70
 H       4.656054    -1.783985    -1.654800      21.96
 C       2.715852     0.788057    -2.575249      60.15
 H       2.322582     0.499144    -3.660342      24.29
 C       2.407259     2.476183    -0.762835      57.98
 C       1.697135     3.598776    -0.269639     103.25
 H       1.900534     4.383558    -0.858938      23.66
 O       1.934698     3.955770     1.193807     309.07
 H       2.617267     4.542678     1.438703      31.47
 C       0.084320     3.542502    -0.402778      81.78
 H       0.096708     3.477312    -1.549233      18.66
 C      -0.585608     4.946776    -0.106438      91.27
 O       0.267895     6.129289    -0.583681     265.57
 H       0.245199     6.119124    -1.546179      31.79
 H      -0.760898     4.995350     1.039945      24.96
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 H      -1.614764     5.107079    -0.477259      24.61
 C      -1.579058    -0.671922    -0.333345      49.91
 H      -0.984914    -1.701973    -0.426142      18.03
 C      -3.303242     0.663716    -0.885724      52.81
 H      -4.210199     0.696969    -1.648202      20.15
 C      -2.580774     1.836165    -0.585970      21.11
 O      -2.949220     3.076318    -1.068009     222.78
 C      -4.290477     3.439993    -1.282630      97.38
 H      -4.927611     2.523990    -0.662534      23.36
 H      -4.264286     4.422096    -0.513274      23.07
 H      -4.655280     3.836067    -2.315430      24.15
 C      -1.295617     1.661023    -0.076667      21.62
 O      -0.509014     2.600365     0.445210     240.94
 C      -0.727721     0.309972     0.075414      25.86
 H       0.454880     0.299755     0.258580      18.50
 C      -2.845635    -0.625211    -0.754526      32.29
 C      -3.522852    -1.927819    -1.120362      77.02
 H      -4.514647    -1.532657    -1.480327      22.56
 O      -2.625911    -2.650413    -1.941537     221.64
 H      -2.786763    -3.695055    -1.976298      17.64
 C      -4.060796    -2.578998     0.253604      90.89
 H      -3.237364    -2.841018     0.945876      21.16
 O      -4.995571    -1.658295     0.790867     356.21
 H      -4.706193    -1.531621     1.740849      26.25
 C      -5.007092    -3.811043    -0.108912      75.83
 O      -4.287350    -4.815311    -0.951435     302.40
 H      -3.498060    -5.309778    -0.486466      25.33
 H      -5.985168    -3.592398    -0.570484      26.39
 H      -5.212152    -4.406329     0.993419      24.86
55
name = lig-etoh-frame_664
 C       2.329973     2.071619    -2.125409      22.79
 H       1.806818     2.812069    -2.765968      18.44
 C       3.272060     1.680080     0.028480      34.77
 H       3.329640     2.099533     1.007788      15.23
 C       3.733390     0.409942    -0.384464      24.71
 O       4.613216    -0.322044     0.409574     263.01
 C       6.052602     0.050009     0.347696     101.01
 H       6.219122     0.781895    -0.493516      29.56
 H       6.778159    -0.821681     0.227839      26.65
 H       6.187652     0.341730     1.365321      27.21
 C       3.515797    -0.128851    -1.777127      18.78
 O       3.889278    -1.360844    -2.235766     189.21
 H       4.653149    -1.690650    -1.752982      23.51
 C       2.805159     0.765890    -2.612893      53.86
 H       2.521752     0.350989    -3.629520      22.36
 C       2.452415     2.511932    -0.762873      63.75
 C       1.659016     3.647027    -0.198017     100.49
 H       1.895677     4.756718    -0.858110      17.58
 O       1.931563     3.985601     1.160915     250.56
 H       2.924971     4.360156     1.250340      27.97
 C       0.116172     3.553650    -0.394298      79.07
 H       0.099855     3.215146    -1.421104      18.83
 C      -0.600365     4.978010    -0.090644      95.78
 O       0.238745     6.149365    -0.619344     224.15
 H       0.152452     5.895016    -1.637222      27.97
 H      -0.999234     4.865542     0.920425      25.46
 H      -1.584664     5.233247    -0.511879      23.82
 C      -1.520776    -0.676495    -0.324522      49.46
 H      -1.150376    -1.646884    -0.682229      18.94
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 C      -3.386810     0.749764    -0.980389      50.34
 H      -4.177314     0.854342    -1.696365      18.96
 C      -2.570222     1.791527    -0.550574      22.06
 O      -2.904710     3.046746    -1.056170     210.48
 C      -4.325165     3.438751    -1.238488     125.36
 H      -4.932839     2.817098    -0.792128      30.70
 H      -4.559510     4.353045    -0.534781      26.40
 H      -4.844373     3.596445    -2.151279      27.63
 C      -1.269502     1.599624    -0.079480      30.38
 O      -0.513012     2.617733     0.434976     241.23
 C      -0.763651     0.383052     0.090187      54.30
 H       0.240967     0.180273     0.424601      19.74
 C      -2.805970    -0.619429    -0.828921      19.97
 C      -3.514094    -1.902358    -1.092053      80.18
 H      -4.543404    -1.908406    -1.639910      22.09
 O      -2.593582    -2.606849    -1.935941     221.87
 H      -3.121764    -3.492311    -1.674510      17.51
 C      -4.084410    -2.656572     0.225885      93.05
 H      -3.326243    -3.054453     0.939176      21.20
 O      -5.039010    -1.668980     0.742629     345.89
 H      -4.650797    -1.369410     1.711148      23.65
 C      -5.007368    -3.809738    -0.067064      96.27
 O      -4.278750    -4.851603    -0.969015     283.95
 H      -3.719689    -5.335782    -0.239748      26.04
 H      -5.947485    -3.585163    -0.601053      27.90
 H      -5.208080    -4.322271     0.891399      28.59
55
name = lig-etoh-frame_665
 C       2.285610     2.057296    -2.061212     107.60
 H       1.843795     2.630716    -2.916037      28.23
 C       3.239136     1.632475     0.057169      50.89
 H       3.550101     2.023630     1.073401      22.17
 C       3.780471     0.441990    -0.401664      20.21
 O       4.606051    -0.269753     0.348223     259.67
 C       6.050865     0.129227     0.373750      89.99
 H       6.230900     0.834414    -0.420961      26.07
 H       6.444748    -0.833938    -0.142527      22.51
 H       6.190684     0.452617     1.432420      24.54
 C       3.521803    -0.098286    -1.754873      10.68
 O       3.849178    -1.412738    -2.286787     138.67
 H       4.860050    -1.626204    -1.736150      20.56
 C       2.879439     0.771251    -2.635827      46.83
 H       2.710877     0.365779    -3.667087      17.14
 C       2.513724     2.489274    -0.804173      28.47
 C       1.623815     3.781763    -0.148766     109.71
 H       1.845233     4.595806    -0.693996      20.64
 O       1.957137     4.022107     1.148313     314.28
 H       2.934983     3.992825     1.015210      27.93
 C       0.147598     3.610563    -0.418739      65.12
 H      -0.121825     3.076363    -1.383259      19.05
 C      -0.609964     5.014590    -0.110523      87.69
 O       0.193210     6.145460    -0.635517     245.07
 H       0.108379     5.916060    -1.637791      26.97
 H      -0.795655     5.035017     1.046487      23.53
 H      -1.508293     5.015645    -0.804698      21.35
 C      -1.464674    -0.756763    -0.346584      36.21
 H      -1.017887    -1.746259    -0.567279      17.88
 C      -3.434224     0.748698    -1.066550      45.17
 H      -4.336669     1.060672    -1.678103      20.28
 C      -2.607465     1.760563    -0.581175      16.76
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 O      -2.876283     3.060220    -1.052653     176.57
 C      -4.343170     3.442596    -1.143518      94.84
 H      -5.207534     2.591379    -0.670624      25.12
 H      -4.762491     4.502302    -0.713994      24.55
 H      -4.661185     3.348174    -2.284003      24.88
 C      -1.254917     1.609002    -0.052541      28.22
 O      -0.512242     2.646453     0.457939     228.08
 C      -0.768878     0.382423     0.106306      42.29
 H       0.188709     0.201251     0.591924      19.25
 C      -2.828038    -0.527695    -0.882732      21.14
 C      -3.542452    -1.868787    -1.072701      85.80
 H      -4.368951    -1.921455    -1.796393      21.62
 O      -2.585138    -2.622028    -1.916652     244.00
 H      -2.992988    -3.457991    -1.799546      24.89
 C      -4.115996    -2.697811     0.186089      96.28
 H      -3.357913    -3.055878     0.935632      21.42
 O      -5.065527    -1.684537     0.722128     345.51
 H      -4.651316    -1.112274     1.580027      22.79
 C      -4.989359    -3.853102    -0.072215      86.84
 O      -4.275686    -4.877812    -0.957867     296.65
 H      -3.876182    -5.409626    -0.320736      30.02
 H      -5.865497    -3.485621    -0.607406      27.68
 H      -5.354325    -4.358900     1.019246      25.62
55
name = lig-etoh-frame_666
 C       2.273333     1.982769    -2.105853      83.66
 H       1.731713     2.557638    -2.975045      23.97
 C       3.217098     1.612414     0.097936      67.19
 H       3.705963     1.782204     1.046145      25.39
 C       3.808804     0.464542    -0.480921      30.86
 O       4.627903    -0.252851     0.330225     257.29
 C       6.005113     0.168193     0.361015     101.61
 H       6.212167     1.096438    -0.268460      26.54
 H       6.422397    -0.698699    -0.039328      25.47
 H       6.504134     0.475399     1.366102      26.94
 C       3.515906    -0.054888    -1.740028      11.22
 O       3.844012    -1.432615    -2.294341     237.70
 H       4.634845    -1.706891    -2.009452      29.22
 C       2.917551     0.814682    -2.611600      26.19
 H       2.854898     0.576146    -3.789803      17.04
 C       2.522476     2.493244    -0.792327      21.37
 C       1.608512     3.836773    -0.177441      88.87
 H       2.008360     4.815616    -0.949025      14.94
 O       2.003958     4.054147     1.170221     338.08
 H       2.954998     3.881354     1.198029      26.91
 C       0.127989     3.669419    -0.437972      75.69
 H      -0.118138     3.394007    -1.467456      18.68
 C      -0.603909     5.033355    -0.165863     112.99
 O       0.138797     6.137033    -0.641977     292.99
 H       0.162090     6.149944    -1.632988      31.23
 H      -0.575685     5.301787     0.859156      24.77
 H      -1.483808     4.767918    -0.721574      23.42
 C      -1.466918    -0.807149    -0.402938      35.63
 H      -0.896286    -1.822541    -0.158738      17.03
 C      -3.434585     0.713821    -1.134473      50.49
 H      -4.484182     1.012978    -1.471744      22.67
 C      -2.620970     1.781252    -0.652032       5.73
 O      -2.894268     3.108762    -1.028580     215.38
 C      -4.400719     3.394719    -1.083686     119.55
 H      -4.893619     2.719927    -0.598728      30.13
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 H      -4.576402     4.521969    -0.839363      25.70
 H      -4.343360     3.290600    -2.124962      25.64
 C      -1.298978     1.684777    -0.024863      -4.72
 O      -0.510337     2.683051     0.515321     208.59
 C      -0.737699     0.273927     0.124002       8.55
 H       0.268796     0.349041     0.759586      15.72
 C      -2.847992    -0.488966    -0.903835      27.63
 C      -3.574568    -1.861386    -1.095224      64.95
 H      -4.425983    -1.556947    -1.865595      20.31
 O      -2.570249    -2.663349    -1.889415     176.51
 H      -2.727063    -3.732073    -2.098541      18.40
 C      -4.127039    -2.656691     0.172941      95.42
 H      -3.305893    -2.836858     0.874909      22.60
 O      -5.083070    -1.694096     0.715998     417.62
 H      -4.685553    -1.247752     1.368490      32.32
 C      -4.983859    -3.941238    -0.103307      93.07
 O      -4.293550    -4.886610    -0.932561     279.41
 H      -3.783716    -5.678474    -0.419017      24.28
 H      -5.848241    -3.492435    -0.656654      27.22
 H      -5.476508    -4.277826     0.856709      26.85
55
name = lig-etoh-frame_667
 C       2.274793     1.938980    -2.177010      64.22
 H       1.669410     2.538815    -2.789547      23.40
 C       3.217419     1.610256     0.092199      45.50
 H       3.636639     1.740323     1.113729      24.05
 C       3.820295     0.477886    -0.539369      34.44
 O       4.660383    -0.259150     0.352422     265.78
 C       5.981260     0.215236     0.336565     109.80
 H       6.083137     1.104698    -0.200033      27.85
 H       6.833837    -0.622943     0.035999      24.12
 H       6.501856     0.334846     1.297148      28.18
 C       3.535972    -0.072400    -1.768327       6.12
 O       3.811579    -1.398027    -2.289187     187.21
 H       4.811387    -1.871481    -2.055438      22.71
 C       2.920151     0.871919    -2.624342      42.10
 H       2.905629     0.744610    -3.631356      19.17
 C       2.461315     2.508209    -0.753027      13.60
 C       1.685099     3.846784    -0.282968      82.26
 H       1.957166     4.612890    -0.842657      17.79
 O       2.038036     4.086051     1.195023     330.28
 H       3.030257     3.960561     1.462596      26.82
 C       0.098483     3.740679    -0.426340      78.73
 H       0.025493     3.642098    -1.549774      16.83
 C      -0.583347     5.028602    -0.230980      98.02
 O       0.091431     6.163231    -0.659461     274.58
 H       0.167589     6.301605    -1.711893      27.70
 H      -0.641004     5.360927     0.908332      22.55
 H      -1.729489     4.865448    -0.421904      22.04
 C      -1.469781    -0.805330    -0.420195      43.63
 H      -1.214432    -1.739199    -0.047345      18.77
 C      -3.402620     0.708059    -1.161075      46.08
 H      -4.457260     0.695349    -1.342174      24.18
 C      -2.575664     1.858134    -0.730044       2.71
 O      -2.936954     3.165124    -0.972805     200.71
 C      -4.386756     3.368828    -1.071732      85.55
 H      -4.916015     2.617969    -0.211452      22.41
 H      -4.310400     4.582973    -0.857787      22.65
 H      -4.572584     3.242806    -2.237483      22.96
 C      -1.349213     1.669650    -0.003793     -14.11
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 O      -0.511908     2.728909     0.562778     187.69
 C      -0.729520     0.247138     0.140769      22.30
 H       0.146618     0.237754     0.656054      16.62
 C      -2.827612    -0.593581    -0.900157      12.62
 C      -3.615754    -1.869548    -1.176472      71.58
 H      -4.464606    -1.489829    -1.698627      22.48
 O      -2.539435    -2.720123    -1.877099     212.26
 H      -2.793759    -3.637792    -2.072848      20.57
 C      -4.141937    -2.576049     0.153130      83.40
 H      -3.214961    -2.632536     0.813524      20.00
 O      -5.114908    -1.718535     0.696879     347.91
 H      -4.536381    -1.252910     1.619104      19.47
 C      -4.972984    -3.980374    -0.160450      84.95
 O      -4.310586    -4.925406    -0.911433     313.28
 H      -3.730279    -5.617094    -0.503347      26.20
 H      -5.813929    -3.676488    -0.789041      26.61
 H      -5.508025    -4.404112     0.896974      25.01
55
name = lig-etoh-frame_668
 C       2.265914     2.008560    -2.140658      50.52
 H       1.518338     2.678589    -2.837704      20.05
 C       3.222944     1.639046     0.037865      15.35
 H       3.358079     1.864824     1.106737      20.52
 C       3.838966     0.458105    -0.529593      28.35
 O       4.681611    -0.281928     0.379940     271.66
 C       6.038724     0.223220     0.318752      89.03
 H       6.015339     1.183091    -0.311593      22.97
 H       6.776771    -0.350111    -0.124420      25.50
 H       6.185285     0.342532     1.490082      23.63
 C       3.578231    -0.107460    -1.828469      17.39
 O       3.792751    -1.346448    -2.275657     159.42
 H       4.757887    -1.723035    -2.012464      23.74
 C       2.924151     0.871265    -2.660501      50.85
 H       2.874864     0.671263    -3.908729      15.68
 C       2.373158     2.478375    -0.741390      43.75
 C       1.783272     3.765951    -0.310795      81.21
 H       2.097450     4.843574    -1.002974      17.19
 O       2.053447     4.116563     1.201908     300.46
 H       3.019670     4.176040     1.353277      28.10
 C       0.112271     3.784132    -0.418519      66.45
 H       0.032493     3.468893    -1.487627      17.50
 C      -0.626687     5.058798    -0.195175     118.01
 O       0.061777     6.238203    -0.702672     315.70
 H      -0.009360     6.106766    -1.653352      32.23
 H      -0.682875     5.093024     0.861027      26.13
 H      -1.660210     5.162224    -0.349072      25.85
 C      -1.494219    -0.772323    -0.395824      39.54
 H      -1.456805    -1.941967    -0.078046      16.73
 C      -3.305158     0.684720    -1.140993      35.68
 H      -4.455075     0.502972    -1.343234      21.70
 C      -2.521797     1.908239    -0.799615       4.61
 O      -2.981360     3.210822    -0.908318     225.11
 C      -4.349340     3.351272    -1.070610     128.94
 H      -4.886336     2.984747    -0.302039      28.84
 H      -4.436882     4.478315    -0.818112      25.72
 H      -5.019530     3.129722    -1.921053      26.13
 C      -1.340451     1.601934     0.010204       0.18
 O      -0.527203     2.769101     0.566548     151.20
 C      -0.799771     0.322578     0.123356      45.23
 H       0.266819     0.013169     0.631686      15.59
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 C      -2.788034    -0.690383    -0.902123      12.82
 C      -3.616518    -1.894300    -1.246528      62.62
 H      -4.654105    -1.695303    -1.845636      21.28
 O      -2.527982    -2.762907    -1.872780     198.32
 H      -3.079651    -3.614373    -1.902409      18.89
 C      -4.153230    -2.525438     0.104216      89.71
 H      -3.293155    -2.657700     0.732403      22.07
 O      -5.128214    -1.712777     0.723388     395.12
 H      -4.866741    -1.452871     1.568034      30.18
 C      -4.964721    -3.963315    -0.177669      92.82
 O      -4.307277    -4.998356    -0.928571     318.57
 H      -3.645887    -5.436007    -0.345428      27.21
 H      -5.819649    -3.772591    -0.864519      26.16
 H      -5.313998    -4.452697     0.775727      26.69
55
name = lig-etoh-frame_669
 C       2.236676     2.120309    -2.098861      90.67
 H       1.712834     2.607636    -2.790594      22.52
 C       3.223685     1.661463    -0.031501      52.76
 H       3.193224     1.952906     1.016316      14.36
 C       3.850074     0.415722    -0.483998      12.66
 O       4.685488    -0.314264     0.383279     266.77
 C       6.079578     0.265033     0.339416      88.71
 H       6.024205     1.203584    -0.171214      28.98
 H       6.742210    -0.461199    -0.387065      24.35
 H       6.175894     0.455859     1.326454      26.21
 C       3.599084    -0.044923    -1.865043      23.63
 O       3.797411    -1.320825    -2.272183     186.53
 H       4.640574    -1.585303    -1.932397      23.00
 C       2.908462     0.854371    -2.736009      23.56
 H       2.776726     0.609008    -3.667374      21.26
 C       2.316348     2.398391    -0.779411      52.59
 C       1.830813     3.756224    -0.273865     103.47
 H       2.170536     4.458735    -0.849629      29.15
 O       2.062240     4.137160     1.167558     277.46
 H       3.035259     4.419049     1.100643      29.80
 C       0.151452     3.758904    -0.438915      47.70
 H      -0.114552     3.208124    -1.351363      22.59
 C      -0.660444     5.132747    -0.103532      83.01
 O       0.031552     6.314883    -0.737775     220.99
 H      -0.138348     5.983659    -1.724053      26.20
 H      -0.563578     5.014089     1.067770      23.93
 H      -1.713373     5.227940    -0.628122      21.64
 C      -1.551252    -0.809109    -0.333888      46.39
 H      -1.158809    -1.739160    -0.180621      20.14
 C      -3.205775     0.639252    -1.103592      50.33
 H      -4.175582     0.779201    -1.442188      18.78
 C      -2.488478     1.868861    -0.833590       8.41
 O      -2.994865     3.225716    -0.859460     216.22
 C      -4.360314     3.391637    -1.056944     115.00
 H      -4.990961     3.022213    -0.006243      23.41
 H      -4.772944     4.548110    -0.958113      24.53
 H      -5.103059     2.897037    -1.764596      24.08
 C      -1.290022     1.627821    -0.006082      12.47
 O      -0.552762     2.787382     0.540881     170.61
 C      -0.841017     0.364544     0.115067      53.78
 H       0.049240     0.158565     0.494196      19.00
 C      -2.770931    -0.669559    -0.936587      23.16
 C      -3.602975    -1.917169    -1.296298      87.92
 H      -4.343158    -1.912954    -2.033994      23.33
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 O      -2.566840    -2.821960    -1.872081     200.80
 H      -3.211221    -3.694158    -1.732509      16.96
 C      -4.179373    -2.535635     0.041982      77.14
 H      -3.321601    -2.818997     0.751015      20.42
 O      -5.158142    -1.700469     0.730380     321.69
 H      -4.960910    -1.527201     1.803073      23.40
 C      -4.943927    -3.915074    -0.210549      84.55
 O      -4.278394    -5.083882    -0.955828     272.37
 H      -3.505044    -5.244377    -0.237755      24.39
 H      -5.866781    -3.669388    -0.747094      27.09
 H      -5.267276    -4.386947     0.896213      26.27
55
name = lig-etoh-frame_670
 C       2.247591     2.124258    -2.155895      78.76
 H       1.685867     2.847005    -2.984509      19.69
 C       3.237695     1.616788    -0.068886      68.19
 H       3.307098     1.955648     0.991235      16.36
 C       3.828541     0.406354    -0.451575       7.78
 O       4.689133    -0.340910     0.369827     260.46
 C       6.087278     0.279822     0.316603      91.49
 H       6.037620     1.306921    -0.103172      29.53
 H       6.626027    -0.420345    -0.163128      28.36
 H       6.626609     0.465812     1.430667      25.34
 C       3.589049     0.079234    -1.865755      22.34
 O       3.811643    -1.309530    -2.286835     119.92
 H       4.764386    -1.681370    -1.703354      18.91
 C       2.865298     0.901239    -2.710817      43.37
 H       2.547482     0.476632    -3.868992      20.74
 C       2.295813     2.345936    -0.799835      58.99
 C       1.763753     3.728332    -0.181575      94.51
 H       2.421178     4.505497    -1.038161      23.53
 O       2.084925     4.146012     1.098449     248.28
 H       2.995080     4.622482     1.039778      27.28
 C       0.170290     3.714288    -0.450598      47.50
 H      -0.184577     3.244013    -1.416668      21.79
 C      -0.654368     5.193790    -0.037107      97.42
 O      -0.007675     6.366906    -0.761423     241.45
 H      -0.059001     6.175712    -1.748620      29.47
 H      -0.611025     5.325360     0.987308      26.95
 H      -1.547971     4.994075    -0.525875      24.34
 C      -1.571882    -0.829682    -0.251123      41.98
 H      -0.715858    -1.681919    -0.237554      18.14
 C      -3.146679     0.666378    -1.092655      59.93
 H      -4.076427     1.075051    -1.684204      17.27
 C      -2.450499     1.802568    -0.801846      16.75
 O      -2.988509     3.206672    -0.835487     185.09
 C      -4.488607     3.430596    -0.966826     116.23
 H      -4.760832     3.099576    -0.071214      28.11
 H      -4.720273     4.529098    -1.212006      26.07
 H      -4.727689     2.717137    -1.817749      23.63
 C      -1.250494     1.763028    -0.064797       5.92
 O      -0.574878     2.781820     0.514776     201.21
 C      -0.877099     0.342605     0.105557      11.00
 H       0.242366     0.323141     0.608311      16.82
 C      -2.781904    -0.641991    -0.985810      39.38
 C      -3.551939    -1.928441    -1.311426      77.28
 H      -4.218262    -1.818732    -2.319781      20.41
 O      -2.640320    -2.915608    -1.856516     268.64
 H      -2.908883    -3.783509    -1.806434      24.69
 C      -4.204015    -2.582782     0.004836      84.89
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 H      -3.378967    -2.821789     0.638009      22.93
 O      -5.184875    -1.682638     0.728794     303.16
 H      -4.830111    -1.730823     1.761396      22.66
 C      -4.941851    -3.885801    -0.235153      83.64
 O      -4.239213    -5.124270    -0.954875     296.60
 H      -3.465805    -5.390538    -0.468185      28.75
 H      -5.920124    -3.616564    -0.656139      26.89
 H      -5.179110    -4.138495     0.851678      27.80
55
name = lig-etoh-frame_671
 C       2.246344     2.101429    -2.295466      39.31
 H       1.793312     2.822069    -2.807555      17.92
 C       3.238703     1.559228    -0.036422      78.37
 H       3.558179     1.887465     0.941625      17.94
 C       3.800430     0.415589    -0.470856      11.84
 O       4.706854    -0.348225     0.354860     256.50
 C       6.080572     0.300668     0.349562     103.31
 H       6.052328     1.292009    -0.168762      30.67
 H       6.790829    -0.512878    -0.207705      25.40
 H       6.673769     0.268757     1.163410      29.22
 C       3.583256     0.126896    -1.837304      18.92
 O       3.857107    -1.276028    -2.283545     222.09
 H       4.485078    -1.640947    -1.778816      24.62
 C       2.785243     0.963604    -2.705983      50.28
 H       2.541178     0.597289    -3.573299      26.09
 C       2.307032     2.342679    -0.796827      50.21
 C       1.686526     3.701173    -0.199230     110.83
 H       2.070976     4.330815    -0.824149      27.97
 O       2.103963     4.156408     1.047062     299.18
 H       2.961237     4.548632     1.106933      31.05
 C       0.159025     3.720014    -0.418979      71.10
 H      -0.018082     3.599713    -1.498437      22.42
 C      -0.575607     5.220674    -0.064048      86.97
 O      -0.052450     6.406480    -0.760794     238.05
 H      -0.020260     6.277319    -1.714916      31.57
 H      -0.679806     5.678467     1.015110      24.05
 H      -1.677506     4.820516    -0.286163      22.19
 C      -1.521063    -0.822329    -0.181301      41.88
 H      -0.880531    -1.643897    -0.292577      20.21
 C      -3.177939     0.733992    -1.155432      51.94
 H      -3.974680     0.919677    -1.799958      18.01
 C      -2.418177     1.839030    -0.716125      20.29
 O      -2.976034     3.174101    -0.828031     157.14
 C      -4.568669     3.426006    -0.906995     100.09
 H      -4.963795     3.126039     0.177436      23.99
 H      -4.494465     4.476362    -1.532232      23.67
 H      -4.585765     2.749419    -1.744055      23.15
 C      -1.221534     1.803856    -0.130269      19.48
 O      -0.570456     2.785440     0.496223     223.85
 C      -0.847735     0.372655     0.128871      17.82
 H       0.078233     0.335826     0.613505      20.52
 C      -2.764213    -0.674363    -1.003732       5.51
 C      -3.537098    -1.944475    -1.357350      88.20
 H      -4.223483    -1.569771    -2.054581      25.02
 O      -2.671228    -2.996910    -1.847084     232.12
 H      -2.870940    -4.040378    -1.789114      16.98
 C      -4.225935    -2.592613    -0.045520      80.26
 H      -3.284605    -2.727256     0.594952      21.74
 O      -5.179311    -1.692058     0.713825     341.11
 H      -4.808472    -1.679778     1.574162      27.79
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 C      -4.939344    -3.889528    -0.256609      77.69
 O      -4.228669    -5.115539    -0.952724     253.67
 H      -3.431813    -5.630465    -0.498915      23.79
 H      -5.911075    -3.772955    -0.779644      26.21
 H      -5.194042    -4.197019     0.911850      25.95
55
name = lig-etoh-frame_672
 C       2.222917     2.137261    -2.290584      37.15
 H       1.653164     2.938462    -2.975773      15.51
 C       3.193682     1.565939     0.030605      53.52
 H       3.674663     1.889118     0.985088      21.50
 C       3.813591     0.396826    -0.521542      23.02
 O       4.730438    -0.333677     0.336939     261.20
 C       6.082913     0.261778     0.321499      97.00
 H       6.085247     1.215428    -0.167508      29.38
 H       6.660939    -0.261479    -0.371527      27.85
 H       6.540023     0.197573     1.483283      24.72
 C       3.567573     0.079567    -1.822560      19.29
 O       3.875526    -1.190074    -2.300765     173.45
 H       4.568484    -1.659220    -1.601109      19.19
 C       2.758987     0.942646    -2.694694      49.94
 H       2.551110     0.529878    -3.852445      22.83
 C       2.348931     2.362094    -0.813555      85.46
 C       1.623804     3.632799    -0.255317      83.46
 H       1.799674     4.655983    -1.141795      22.54
 O       2.095154     4.156831     1.041493     247.28
 H       3.140977     4.314719     1.022764      25.91
 C       0.137361     3.801496    -0.342529      85.72
 H       0.051775     3.838461    -1.472502      17.64
 C      -0.516117     5.221235    -0.099093     113.52
 O      -0.100180     6.436375    -0.750762     218.28
 H      -0.064657     6.197163    -1.791433      28.74
 H      -0.512645     5.612502     0.890870      25.70
 H      -1.551985     5.040358    -0.155089      25.59
 C      -1.495624    -0.762383    -0.173724      41.04
 H      -1.082461    -1.881763    -0.165116      17.64
 C      -3.200999     0.720819    -1.237127      32.73
 H      -4.124525     0.767931    -1.925447      22.46
 C      -2.490170     1.937308    -0.659943      -0.46
 O      -2.973235     3.153103    -0.815322     156.22
 C      -4.543714     3.387598    -0.881018     106.97
 H      -5.255569     3.409688    -0.049180      27.46
 H      -4.528847     4.346032    -1.318131      27.52
 H      -5.032105     2.654631    -1.612246      25.50
 C      -1.171045     1.706420    -0.154774      26.02
 O      -0.535821     2.818102     0.471569     190.83
 C      -0.800163     0.443496     0.158111      45.43
 H       0.200108     0.257200     0.743824      20.26
 C      -2.694932    -0.674833    -0.966643      -4.31
 C      -3.549315    -1.963205    -1.376315      71.45
 H      -4.477447    -1.495395    -1.976184      22.70
 O      -2.662627    -3.072546    -1.864771     197.69
 H      -3.254353    -3.870183    -1.581772      16.75
 C      -4.212247    -2.549199    -0.083278      87.30
 H      -3.356099    -2.699548     0.537419      22.17
 O      -5.159645    -1.727733     0.654578     329.12
 H      -4.683195    -1.399595     1.702200      20.61
 C      -4.931629    -3.955757    -0.250958     102.36
 O      -4.223908    -5.082916    -0.956376     265.14
 H      -3.682149    -5.651187    -0.288016      25.37
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 H      -5.734246    -3.908864    -0.943867      26.74
 H      -5.285406    -4.388875     0.759364      27.40
55
name = lig-etoh-frame_673
 C       2.188533     2.194910    -2.205890      51.96
 H       1.662818     2.710245    -2.964975      20.17
 C       3.153481     1.584459     0.064736      38.23
 H       3.473598     1.945704     1.034643      23.38
 C       3.840212     0.416655    -0.516477      25.89
 O       4.740457    -0.312331     0.302708     266.72
 C       6.085975     0.212420     0.312094      99.56
 H       6.054714     1.352065     0.062606      26.67
 H       6.718466    -0.313042    -0.528392      24.32
 H       6.231228     0.217351     1.295869      27.35
 C       3.510093     0.011837    -1.854842       9.75
 O       3.912604    -1.115555    -2.327418     163.07
 H       4.543969    -1.559327    -1.533569      20.57
 C       2.755602     0.860490    -2.727343      57.78
 H       2.736426     0.623446    -3.753797      24.71
 C       2.382018     2.420689    -0.838010      53.35
 C       1.621796     3.662777    -0.338784     107.62
 H       1.740767     4.408898    -1.039260      27.27
 O       2.098015     4.144234     1.034038     324.04
 H       3.054103     3.983141     0.895164      27.95
 C       0.115837     3.896570    -0.306446      97.07
 H      -0.173825     3.645993    -1.345845      21.18
 C      -0.471095     5.234430    -0.071882     106.83
 O      -0.134525     6.450941    -0.778339     258.86
 H      -0.161278     6.189188    -1.690094      31.92
 H      -0.171768     5.362898     1.054227      23.78
 H      -1.612869     5.204549    -0.301576      22.55
 C      -1.481623    -0.716903    -0.216310      56.35
 H      -1.320455    -1.706580     0.248997      20.30
 C      -3.186302     0.674361    -1.295838      42.28
 H      -4.143319     0.720799    -1.816387      25.36
 C      -2.597497     1.906345    -0.662852     -15.02
 O      -3.027694     3.180780    -0.791132     189.56
 C      -4.493100     3.318051    -0.907896     118.55
 H      -5.190422     3.551005     0.022301      25.65
 H      -4.637871     4.550206    -1.198929      24.10
 H      -5.290048     2.721136    -1.350810      26.06
 C      -1.161601     1.668205    -0.151552       1.23
 O      -0.506409     2.844527     0.445048     172.57
 C      -0.705007     0.427187     0.205915      44.97
 H       0.241232     0.293286     0.805957      20.42
 C      -2.641931    -0.620548    -0.929943      17.86
 C      -3.564439    -1.940609    -1.369443      76.22
 H      -4.328963    -1.775979    -2.066216      24.03
 O      -2.684196    -3.119421    -1.885557     219.60
 H      -3.296384    -3.783713    -1.593355      20.81
 C      -4.185700    -2.522807    -0.078446      87.15
 H      -3.322600    -2.784659     0.620137      20.84
 O      -5.122144    -1.747715     0.612678     426.97
 H      -4.752456    -1.372482     1.286369      34.79
 C      -4.925810    -4.034900    -0.268028      87.97
 O      -4.211597    -5.051447    -0.947018     297.11
 H      -3.830734    -5.518112    -0.238352      28.38
 H      -5.734726    -3.766588    -1.042635      26.07
 H      -5.402075    -4.464523     0.747336      26.39
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name = lig-etoh-frame_674
 C       2.210266     2.117580    -2.150254      49.51
 H       1.584458     2.722669    -2.876759      21.70
 C       3.137028     1.586836     0.035763      38.11
 H       3.162376     1.941959     1.095878      20.90
 C       3.823522     0.493273    -0.479677      40.47
 O       4.721358    -0.301453     0.245289     246.38
 C       6.074751     0.207156     0.261973     102.01
 H       6.047951     1.250140     0.254576      28.16
 H       6.817261    -0.371943    -0.303765      25.61
 H       6.411831     0.042746     1.447556      25.08
 C       3.419023     0.026747    -1.862235      21.36
 O       3.989835    -1.115759    -2.365889     225.67
 H       4.475405    -1.466067    -1.726142      30.08
 C       2.740901     0.858797    -2.703678      58.32
 H       2.799661     0.624344    -3.867951      20.85
 C       2.377858     2.496884    -0.833453      40.31
 C       1.636601     3.740402    -0.356318      85.85
 H       2.162601     4.583220    -1.240085      20.23
 O       2.101666     4.109797     0.996697     320.65
 H       3.057769     3.930701     0.987105      26.50
 C       0.090745     3.891517    -0.388928      84.18
 H      -0.362139     3.483936    -1.309907      21.37
 C      -0.472823     5.285548     0.028996     112.47
 O      -0.139927     6.460062    -0.805761     233.39
 H      -0.250073     6.184939    -1.790323      27.87
 H      -0.069381     5.302888     1.029332      25.29
 H      -1.515190     5.142631    -0.147828      24.46
 C      -1.446200    -0.685647    -0.214236      46.57
 H      -1.326170    -1.537074     0.503410      19.26
 C      -3.152237     0.660782    -1.304985      67.29
 H      -4.153522     0.711984    -1.730144      25.20
 C      -2.628333     1.764608    -0.699267      -6.91
 O      -3.121420     3.207160    -0.769058     185.92
 C      -4.500916     3.358651    -0.898297     133.08
 H      -4.572633     3.404618     0.217541      23.74
 H      -4.617912     4.267014    -1.339724      28.42
 H      -5.126514     2.592424    -1.450782      25.93
 C      -1.212672     1.732649    -0.130253     -21.55
 O      -0.504356     2.841090     0.450264     161.38
 C      -0.627385     0.371402     0.235814      13.90
 H       0.293300     0.342746     0.831711      19.13
 C      -2.659448    -0.571761    -0.954330      24.82
 C      -3.517710    -1.925494    -1.330445      58.04
 H      -4.187556    -1.847453    -2.305055      19.05
 O      -2.715107    -3.109206    -1.906095     177.47
 H      -3.160715    -4.149565    -1.712261      13.67
 C      -4.138434    -2.570481    -0.029380      95.74
 H      -3.307366    -2.801753     0.626519      22.15
 O      -5.113625    -1.762817     0.539796     340.11
 H      -4.596475    -1.178815     1.377054      22.69
 C      -4.959052    -4.043757    -0.317146      89.26
 O      -4.196427    -5.034577    -0.937448     276.04
 H      -3.598608    -5.604673    -0.228098      22.42
 H      -5.779925    -3.641694    -0.858448      28.24
 H      -5.502779    -4.328849     0.696570      27.53
55
name = lig-etoh-frame_675
 C       2.229896     2.007418    -2.155354      45.87
 H       1.605234     2.778220    -2.681202      22.22
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 C       3.107025     1.640651     0.008943      56.67
 H       3.006894     1.763057     1.088740      21.25
 C       3.765722     0.548199    -0.492272      43.59
 O       4.688742    -0.300803     0.178917     245.57
 C       6.077526     0.192004     0.309152     108.08
 H       6.150327     1.359592     0.172997      26.50
 H       6.835762    -0.369638    -0.321765      25.66
 H       6.547184    -0.161502     1.148151      28.53
 C       3.386476     0.055059    -1.811002      15.36
 O       4.054069    -1.119927    -2.428116     132.24
 H       4.739215    -1.610186    -1.607565      21.85
 C       2.705897     0.910410    -2.685086      62.66
 H       2.682126     0.661330    -3.792566      19.30
 C       2.357085     2.521899    -0.813410      22.73
 C       1.707269     3.865587    -0.383583      96.10
 H       2.190954     4.588975    -1.010372      21.40
 O       2.092511     4.069621     0.950942     295.01
 H       3.119825     4.124080     1.116708      25.12
 C       0.065437     3.838169    -0.523720      55.61
 H      -0.295444     3.688521    -1.564945      21.34
 C      -0.476680     5.316724     0.100253      84.55
 O      -0.128970     6.459525    -0.824473     193.78
 H      -0.329022     6.119102    -1.779314      27.87
 H      -0.108203     5.601882     1.133507      23.29
 H      -1.619173     5.085171     0.277195      23.17
 C      -1.407757    -0.678399    -0.165109      31.22
 H      -1.252433    -1.647867     0.471471      18.84
 C      -3.165922     0.651795    -1.310338      61.07
 H      -4.212871     0.720891    -1.769627      25.65
 C      -2.551653     1.740956    -0.711335       5.09
 O      -3.141990     3.163702    -0.777200     185.07
 C      -4.537491     3.389193    -0.841883     118.74
 H      -4.680847     3.324789     0.199075      25.21
 H      -4.751920     4.334068    -1.694221      23.37
 H      -4.813421     2.508514    -1.436470      25.07
 C      -1.263084     1.763172    -0.079198      -1.76
 O      -0.524735     2.819652     0.480748     158.29
 C      -0.630610     0.406809     0.206607      10.52
 H       0.370127     0.337226     0.878476      18.07
 C      -2.667645    -0.615287    -0.994523      13.66
 C      -3.450361    -1.961378    -1.307504      75.36
 H      -4.098367    -1.586633    -2.072908      22.12
 O      -2.719884    -3.092305    -1.931409     260.74
 H      -3.021942    -3.884636    -1.731130      23.97
 C      -4.103267    -2.661492    -0.007205      87.78
 H      -3.230564    -2.826401     0.694017      20.58
 O      -5.105491    -1.743960     0.498190     358.45
 H      -4.719415    -1.250245     1.337183      26.13
 C      -4.981899    -3.959993    -0.331797      80.72
 O      -4.172075    -5.058163    -0.927747     333.72
 H      -3.474288    -5.485352    -0.431176      27.85
 H      -5.902047    -3.684715    -0.966737      25.71
 H      -5.456651    -4.278978     0.701868      26.01
55
name = lig-etoh-frame_676
 C       2.180237     2.049328    -2.129563      43.64
 H       1.676455     2.696517    -2.808561      24.85
 C       3.058126     1.729141     0.028662      68.56
 H       3.103023     1.695890     1.118374      22.74
 C       3.712206     0.534291    -0.556770      47.14
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 O       4.659286    -0.296515     0.128590     238.21
 C       6.095297     0.182099     0.332355      91.59
 H       6.242638     1.197455     0.145737      28.70
 H       6.545167    -0.205280    -0.656786      24.52
 H       6.523686    -0.288905     1.344980      25.24
 C       3.441218     0.041875    -1.775334      23.48
 O       4.106890    -1.101522    -2.448325     232.13
 H       4.749773    -1.494353    -1.852005      28.17
 C       2.694141     0.883892    -2.692178      50.74
 H       2.501455     0.673641    -3.742190      20.65
 C       2.337170     2.495894    -0.825780      25.21
 C       1.768668     3.907679    -0.408588      78.37
 H       2.143177     4.987073    -1.047407      19.53
 O       2.079649     4.045944     0.948435     288.05
 H       2.994219     4.382322     0.986765      27.12
 C       0.061094     3.842696    -0.589518      39.93
 H      -0.174478     3.887288    -1.666410      22.17
 C      -0.495379     5.315750     0.134947      83.19
 O      -0.131435     6.432375    -0.827727     187.69
 H      -0.344208     6.105875    -1.680868      32.15
 H       0.017136     5.805754     1.014091      23.05
 H      -1.508708     5.239988     0.524887      25.78
 C      -1.410012    -0.709596    -0.119951      28.83
 H      -1.114726    -1.707911     0.154838      18.30
 C      -3.202761     0.616091    -1.305462      25.15
 H      -4.101570     0.750563    -1.819159      19.03
 C      -2.470160     1.841574    -0.715508       3.76
 O      -3.079658     3.094875    -0.796298     183.03
 C      -4.567652     3.391189    -0.846386     111.54
 H      -5.410344     3.508411     0.069308      25.05
 H      -4.815768     4.153968    -1.392429      29.30
 H      -4.961152     2.455196    -1.297931      24.65
 C      -1.268489     1.724784    -0.011439      24.67
 O      -0.548598     2.814019     0.481644     136.92
 C      -0.680799     0.500839     0.164518      46.96
 H       0.155212     0.384209     0.718005      20.08
 C      -2.609307    -0.712592    -0.990668      -2.08
 C      -3.381485    -2.017971    -1.275356      75.25
 H      -4.316736    -1.464019    -1.812031      23.07
 O      -2.676696    -3.016583    -1.979935     181.97
 H      -3.241871    -3.981745    -1.551475      11.98
 C      -4.092603    -2.714837    -0.017478      91.23
 H      -3.337998    -2.946361     0.753580      22.79
 O      -5.095531    -1.721160     0.471463     366.86
 H      -4.830675    -1.401788     1.330781      30.28
 C      -4.971366    -3.865989    -0.320717      95.86
 O      -4.170131    -5.075862    -0.943276     255.46
 H      -3.414536    -5.382609    -0.307209      25.66
 H      -5.678242    -3.804709    -1.107389      26.78
 H      -5.348363    -4.314608     0.717433      26.81
55
name = lig-etoh-frame_677
 C       2.110793     2.120613    -2.153642      56.08
 H       1.668001     2.686178    -3.063662      23.06
 C       3.055411     1.729887     0.060591      33.93
 H       3.301769     1.927725     1.137635      22.72
 C       3.686933     0.523112    -0.554228      43.14
 O       4.632059    -0.282305     0.113552     229.05
 C       6.091751     0.140393     0.304661      96.75
 H       6.222450     1.313923     0.370661      27.38
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 H       6.437152    -0.176410    -0.626481      26.39
 H       6.345367    -0.250973     1.257377      26.98
 C       3.511692     0.002616    -1.870502      16.03
 O       4.128044    -1.045967    -2.456797     215.73
 H       4.884044    -1.460149    -1.888526      24.25
 C       2.689217     0.832874    -2.663024      64.96
 H       2.315757     0.571921    -3.796092      20.92
 C       2.302786     2.528785    -0.848311      48.94
 C       1.769703     3.911690    -0.448823     100.19
 H       2.000389     4.826645    -1.017184      23.03
 O       2.063712     4.048557     0.972438     309.06
 H       2.932169     4.530904     0.933547      26.41
 C       0.086969     3.926444    -0.536501      39.07
 H      -0.238616     3.792656    -1.603316      22.08
 C      -0.463027     5.318523     0.130339      91.97
 O      -0.152539     6.392022    -0.812045     183.18
 H      -0.377868     6.093910    -1.809847      27.02
 H       0.266613     5.561614     0.922503      23.63
 H      -1.566606     5.357697     0.427010      24.81
 C      -1.443083    -0.734221    -0.121380      49.74
 H      -0.751708    -1.730664    -0.173257      19.14
 C      -3.148650     0.581754    -1.238630      23.08
 H      -4.073031     0.743716    -1.954774      18.44
 C      -2.487189     1.882523    -0.752089       0.06
 O      -3.025556     3.073063    -0.803740     145.55
 C      -4.621811     3.299926    -0.831347      86.11
 H      -5.357574     3.634589    -0.162642      26.64
 H      -4.725118     4.432164    -1.476953      23.46
 H      -5.244057     2.516704    -1.273383      25.18
 C      -1.261084     1.728077     0.031014      22.86
 O      -0.556697     2.839070     0.445571     149.81
 C      -0.768605     0.501234     0.130957      36.90
 H       0.328318     0.478522     0.726528      18.26
 C      -2.539514    -0.760570    -0.943722      19.56
 C      -3.364768    -2.034445    -1.240070      92.05
 H      -4.330677    -1.799493    -1.614023      25.42
 O      -2.642114    -2.973253    -2.020883     285.18
 H      -3.087258    -3.744275    -1.861659      25.32
 C      -4.083349    -2.681836    -0.019798      96.90
 H      -3.462313    -3.071370     0.821855      22.16
 O      -5.075185    -1.701102     0.435940     297.08
 H      -4.885119    -1.640703     1.611211      21.27
 C      -4.929798    -3.863499    -0.310959      93.59
 O      -4.158134    -5.073522    -0.954382     277.19
 H      -3.567724    -5.372805    -0.156442      26.27
 H      -5.615526    -3.672404    -1.192488      27.31
 H      -5.407110    -4.235180     0.624764      29.25
55
name = lig-etoh-frame_678
 C       2.074198     2.113931    -2.251006      23.11
 H       1.608526     2.727042    -2.957369      21.24
 C       3.088603     1.669116     0.047126      32.89
 H       3.422662     2.195606     0.933122      23.32
 C       3.687083     0.526068    -0.517506      20.91
 O       4.610652    -0.268235     0.136524     246.44
 C       6.022636     0.150207     0.258819     104.15
 H       6.086808     1.153602     0.591200      28.18
 H       6.795905    -0.314663    -0.581171      24.54
 H       6.368905    -0.424183     1.198974      26.24
 C       3.541335     0.033525    -1.977563       2.15
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 O       4.153261    -1.010340    -2.472644     154.52
 H       5.032934    -1.412823    -1.852505      19.26
 C       2.630932     0.826831    -2.646248      57.46
 H       2.400427     0.487444    -3.573473      25.29
 C       2.273914     2.590944    -0.871314      57.78
 C       1.680886     3.857746    -0.431142      90.10
 H       2.085777     4.792397    -1.226414      21.37
 O       2.050136     4.080719     0.992380     289.31
 H       2.970974     4.529705     1.090658      26.39
 C       0.098789     4.008661    -0.435551      68.66
 H      -0.324993     3.660267    -1.365196      23.27
 C      -0.393573     5.308056     0.089896     119.38
 O      -0.177059     6.360436    -0.811059     262.24
 H      -0.336897     6.082241    -1.732626      30.05
 H       0.301396     5.205642     0.999414      24.11
 H      -1.480585     5.310788     0.275568      25.67
 C      -1.394584    -0.781661    -0.155229      59.50
 H      -0.695399    -1.496316    -0.213856      22.07
 C      -3.056484     0.573900    -1.164572      59.41
 H      -3.841907     0.578921    -1.823035      21.48
 C      -2.530115     1.785475    -0.773557      14.12
 O      -3.044332     3.111655    -0.808648     137.63
 C      -4.663765     3.266095    -0.892630      98.45
 H      -4.879711     3.666979     0.307363      23.13
 H      -4.477105     4.010124    -1.483117      27.65
 H      -5.256953     2.511151    -1.450892      25.13
 C      -1.294723     1.800037     0.002328      -4.10
 O      -0.540080     2.892139     0.406692     173.21
 C      -0.776007     0.418005     0.164569      27.59
 H       0.137443     0.479667     0.499344      22.06
 C      -2.555412    -0.743482    -0.904478      33.04
 C      -3.368750    -2.033278    -1.189889      71.54
 H      -4.337344    -1.856029    -1.892881      22.37
 O      -2.585041    -2.919972    -2.076733     203.56
 H      -3.022352    -3.953714    -2.126625      19.43
 C      -4.055100    -2.635342     0.027030     104.21
 H      -3.412869    -2.965625     0.883321      23.52
 O      -5.039244    -1.683134     0.451327     361.13
 H      -4.988537    -1.732044     1.306023      32.12
 C      -4.887267    -3.926350    -0.373246      81.65
 O      -4.150148    -5.049002    -0.934792     300.23
 H      -3.684099    -5.511329    -0.261895      28.91
 H      -5.636441    -3.464486    -1.039585      29.15
 H      -5.683963    -4.139626     0.559804      28.29
55
name = lig-etoh-frame_679
 C       2.069454     2.084537    -2.279923      33.95
 H       1.419642     2.778676    -2.936302      18.72
 C       3.100137     1.655933    -0.038652      44.34
 H       3.527761     2.239853     0.814689      21.76
 C       3.710342     0.515993    -0.543055      18.21
 O       4.605995    -0.269098     0.180540     263.92
 C       5.968544     0.116643     0.247514     119.35
 H       6.035599     1.208394     0.580420      27.74
 H       6.742019    -0.103482    -0.399131      28.29
 H       6.364892    -0.582073     1.012985      27.39
 C       3.534747     0.156497    -1.953195       9.31
 O       4.208447    -1.015179    -2.501462     224.33
 H       4.822970    -1.216240    -1.943716      26.99
 C       2.553052     0.852970    -2.660677      49.54
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 H       2.419155     0.361778    -3.802357      24.22
 C       2.272555     2.555889    -0.934089      48.65
 C       1.591550     3.834565    -0.383030      96.27
 H       2.037306     4.603231    -1.095922      23.38
 O       2.039161     4.131472     1.010318     307.52
 H       2.962420     4.363457     1.086960      29.65
 C       0.088186     3.986995    -0.381576      89.90
 H      -0.306603     3.765161    -1.420526      20.65
 C      -0.333111     5.276445     0.077427     117.15
 O      -0.176624     6.366254    -0.809444     268.19
 H      -0.263375     5.966988    -1.736945      29.10
 H       0.076929     5.432088     1.091062      25.06
 H      -1.413071     5.105777     0.315493      24.36
 C      -1.313252    -0.805944    -0.201602      25.52
 H      -0.576611    -1.798543    -0.085265      19.64
 C      -3.001185     0.532574    -1.121173      64.13
 H      -3.968429     0.487742    -1.772800      25.52
 C      -2.525469     1.748673    -0.726632      22.58
 O      -3.108029     3.118381    -0.833405     173.91
 C      -4.639497     3.251238    -0.899082     106.75
 H      -4.533688     3.352162     0.063688      24.39
 H      -4.517216     4.162771    -1.795368      22.28
 H      -5.157737     2.407934    -1.376544      25.58
 C      -1.318514     1.804261    -0.070139      -2.09
 O      -0.520199     2.941050     0.402788     173.52
 C      -0.780008     0.422722     0.211448      15.93
 H       0.433364     0.345501     0.511249      21.84
 C      -2.608581    -0.726341    -0.864575      25.45
 C      -3.401421    -2.018050    -1.205548      72.54
 H      -4.047244    -1.662549    -1.953512      23.06
 O      -2.516440    -2.880335    -2.121850     207.45
 H      -2.922473    -3.876410    -2.224623      20.31
 C      -4.027724    -2.635784     0.088724      99.41
 H      -3.248113    -2.713173     0.866296      22.57
 O      -5.005025    -1.662607     0.445592     287.23
 H      -5.065559    -1.658186     1.578125      24.93
 C      -4.874484    -3.956834    -0.415355      92.97
 O      -4.157309    -5.018025    -0.922774     291.41
 H      -3.678011    -5.684320    -0.280487      24.94
 H      -5.586448    -3.500134    -1.136070      27.97
 H      -5.584471    -4.212772     0.399016      28.04
55
name = lig-etoh-frame_680
 C       2.031035     2.098456    -2.270553      45.51
 H       1.333668     2.589880    -2.907726      19.54
 C       3.098437     1.717106    -0.157802      46.06
 H       3.488274     2.001354     0.810886      20.16
 C       3.749430     0.507666    -0.615742      13.18
 O       4.588621    -0.287055     0.219233     272.79
 C       5.943897     0.094182     0.300889      99.53
 H       6.059724     1.166099     0.548252      28.65
 H       6.537303     0.115328    -0.812258      25.70
 H       6.338731    -0.588213     1.065527      26.73
 C       3.525870     0.239899    -1.892584      15.34
 O       4.218646    -0.979229    -2.542236     147.28
 H       4.971057    -1.220772    -1.722530      19.38
 C       2.508066     0.841427    -2.757912      47.37
 H       2.378005     0.556827    -3.678250      30.14
 C       2.283980     2.453282    -0.975074      44.97
 C       1.569324     3.795666    -0.313246      84.59
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 H       1.982966     4.738274    -1.039922      22.00
 O       2.018558     4.177934     1.025847     249.94
 H       3.036636     4.191338     0.898962      27.22
 C       0.082221     3.875376    -0.412535      89.08
 H      -0.168388     4.003191    -1.468743      20.97
 C      -0.345521     5.279524     0.134485      91.99
 O      -0.162468     6.385203    -0.814947     181.62
 H      -0.135194     5.957578    -1.778793      27.41
 H      -0.054806     5.888125     1.060500      21.97
 H      -1.431797     4.983540     0.311510      23.73
 C      -1.229234    -0.829218    -0.243260      36.99
 H      -0.908557    -1.743169     0.013901      21.79
 C      -3.067742     0.494246    -1.142667      40.84
 H      -4.039959     0.593793    -1.551733      24.82
 C      -2.521049     1.828514    -0.657731       5.07
 O      -3.150723     3.065794    -0.889863     205.98
 C      -4.541735     3.259845    -0.989375     116.35
 H      -4.895065     3.318230     0.296294      23.38
 H      -4.991238     4.069709    -1.444357      27.03
 H      -5.070113     2.290760    -1.170853      25.11
 C      -1.250542     1.750502    -0.109881      12.99
 O      -0.532068     2.943586     0.430961     181.49
 C      -0.707755     0.470417     0.246850      37.40
 H       0.230185     0.353619     0.571000      23.07
 C      -2.582412    -0.784019    -0.794587       4.53
 C      -3.388412    -1.978611    -1.259135      60.70
 H      -4.217166    -1.499751    -1.944647      22.81
 O      -2.451373    -2.840650    -2.141656     235.68
 H      -2.862289    -3.646411    -2.132281      24.95
 C      -4.016796    -2.658108     0.101408      81.42
 H      -3.127984    -2.646191     0.800994      21.63
 O      -4.980704    -1.640910     0.471685     316.45
 H      -5.054266    -1.465511     1.527413      26.96
 C      -4.864697    -3.921851    -0.407304      82.38
 O      -4.145131    -5.024788    -0.942550     285.18
 H      -3.722296    -5.566201    -0.212540      27.01
 H      -5.402143    -3.661331    -1.358922      25.12
 H      -5.529152    -4.442138     0.495544      24.32
55
name = lig-etoh-frame_681
 C       1.965881     2.062024    -2.303840      32.36
 H       1.200380     2.572560    -2.926883      16.87
 C       3.156014     1.736949    -0.236010      56.92
 H       3.236363     1.865438     0.878422      20.48
 C       3.788033     0.550725    -0.631427      12.08
 O       4.537091    -0.305844     0.245281     270.12
 C       5.957395     0.103410     0.313231     103.39
 H       6.063172     1.142210     0.707930      29.10
 H       6.101645     0.085648    -0.661560      31.28
 H       6.517838    -0.571248     1.071857      26.42
 C       3.512602     0.199960    -1.973867      18.01
 O       4.216021    -0.894529    -2.539066     179.49
 H       4.891327    -1.366314    -1.889407      20.54
 C       2.520488     0.868006    -2.788897      61.47
 H       2.285615     0.573240    -3.980888      27.49
 C       2.256765     2.430503    -0.949701      70.54
 C       1.615712     3.755304    -0.284305      96.61
 H       1.878059     4.700453    -0.970189      23.25
 O       2.015377     4.203457     1.030589     259.96
 H       3.005970     4.095361     0.879595      28.49
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 C       0.108724     3.812264    -0.431170      69.85
 H      -0.198603     3.923653    -1.505935      20.59
 C      -0.417067     5.322872     0.194756      88.52
 O      -0.143032     6.393698    -0.829357     208.27
 H      -0.119689     6.117652    -1.741293      31.37
 H       0.009859     5.824648     1.032555      24.30
 H      -1.495900     5.150378     0.257286      25.18
 C      -1.208909    -0.777828    -0.260535      56.69
 H      -0.937290    -1.869819     0.201864      19.88
 C      -3.146548     0.526579    -1.126764      19.34
 H      -4.217665     0.621421    -1.455546      22.32
 C      -2.558848     1.851801    -0.631864     -17.60
 O      -3.146804     3.021601    -0.964472     237.14
 C      -4.504348     3.205724    -0.963566     145.14
 H      -5.111859     3.409031    -0.125062      27.91
 H      -5.208054     4.126004    -1.302792      23.71
 H      -5.008727     2.285143    -1.201711      26.86
 C      -1.137870     1.719375    -0.102820       7.68
 O      -0.580016     2.888847     0.461956     178.10
 C      -0.648231     0.465575     0.227556      34.21
 H       0.410053     0.510036     0.855324      19.27
 C      -2.510478    -0.809689    -0.754332       2.46
 C      -3.348665    -1.932184    -1.319473      70.48
 H      -4.311650    -1.654764    -1.735013      24.32
 O      -2.409758    -2.770552    -2.129923     156.60
 H      -2.948817    -3.820426    -1.986434      15.95
 C      -4.017925    -2.658783     0.051281      90.33
 H      -3.229730    -2.901461     0.761795      23.23
 O      -4.960647    -1.616072     0.504107     373.80
 H      -4.878656    -1.457122     1.405445      31.14
 C      -4.854609    -3.900388    -0.364696      98.65
 O      -4.103695    -5.054027    -0.969851     301.81
 H      -3.666866    -5.426542    -0.214299      29.07
 H      -5.411712    -3.603161    -1.239673      27.39
 H      -5.496483    -4.276507     0.405059      27.92
55
name = lig-etoh-frame_682
 C       1.887290     2.012482    -2.326298      22.07
 H       1.143229     2.617367    -2.902133      18.49
 C       3.240683     1.715660    -0.213406      78.04
 H       3.034855     1.919549     0.828962      19.60
 C       3.817242     0.588031    -0.660656      48.85
 O       4.464945    -0.312619     0.273164     246.21
 C       5.952645     0.125191     0.353457      83.51
 H       6.024366     1.127553     0.871186      27.62
 H       6.251850     0.017138    -0.841136      23.75
 H       6.601745    -0.579993     0.815748      27.91
 C       3.512632     0.117646    -2.082340       4.55
 O       4.202891    -0.817706    -2.553083     199.88
 H       4.756887    -1.351488    -2.018965      23.87
 C       2.559522     0.897577    -2.840145      35.74
 H       2.361828     0.585079    -3.778644      23.02
 C       2.191167     2.484047    -0.938356     101.64
 C       1.656255     3.719556    -0.303197      97.95
 H       1.894387     4.612849    -1.080192      20.25
 O       2.034501     4.196042     1.028803     294.16
 H       2.999041     4.183253     1.146333      30.68
 C       0.114623     3.828540    -0.390911      58.52
 H      -0.293090     3.566363    -1.381751      20.29
 C      -0.483422     5.356086     0.171391      82.08
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 O      -0.117762     6.410612    -0.810720     205.69
 H      -0.240228     6.077070    -1.831107      25.03
 H       0.127679     5.454656     1.163610      23.65
 H      -1.636293     5.404767     0.285007      23.52
 C      -1.202682    -0.750886    -0.217229      60.10
 H      -0.750569    -1.593907     0.184130      21.54
 C      -3.181241     0.592591    -1.041863      43.86
 H      -4.227434     0.457267    -1.404823      23.00
 C      -2.570337     1.745608    -0.645034      -6.74
 O      -3.103723     3.027437    -1.031539     181.18
 C      -4.581365     3.138456    -0.940789     109.00
 H      -5.000034     3.388989     0.236100      23.76
 H      -4.635005     3.999088    -1.690847      24.98
 H      -5.054638     2.282254    -1.505506      24.55
 C      -1.108549     1.723645    -0.092744      -6.11
 O      -0.626445     2.818831     0.484026     175.88
 C      -0.545623     0.432025     0.199512      28.80
 H       0.204909     0.582777     0.936461      18.72
 C      -2.492710    -0.715757    -0.796050      16.96
 C      -3.279842    -1.929114    -1.303539      77.78
 H      -4.261363    -1.686539    -1.840880      22.08
 O      -2.424533    -2.734981    -2.092362     279.90
 H      -2.654337    -3.591249    -2.005167      24.10
 C      -4.013591    -2.646942    -0.029139      89.11
 H      -3.366490    -3.130837     0.788379      19.90
 O      -4.937454    -1.609937     0.515067     311.13
 H      -4.504566    -1.476503     1.630212      19.76
 C      -4.830378    -3.883159    -0.365072      74.18
 O      -4.060622    -5.066298    -0.984364     274.14
 H      -3.407519    -5.467930    -0.237054      24.87
 H      -5.652214    -3.452177    -1.060524      26.48
 H      -5.655583    -4.104873     0.569889      25.84
55
name = lig-etoh-frame_683
 C       1.821759     2.003817    -2.274924      82.49
 H       1.159512     2.534752    -2.924282      25.18
 C       3.226435     1.748110    -0.175458      64.44
 H       3.214111     1.968140     0.920701      18.05
 C       3.827661     0.568259    -0.732813      39.97
 O       4.418988    -0.301912     0.289917     250.18
 C       5.923435     0.133004     0.340196     100.11
 H       5.995384     1.064005     0.850708      28.06
 H       6.473531     0.275474    -0.522581      26.62
 H       6.561825    -0.780151     0.729432      25.25
 C       3.481618     0.161272    -2.069643      30.17
 O       4.217475    -0.814106    -2.649336     155.39
 H       4.791665    -1.449805    -1.832712      23.06
 C       2.616706     0.913737    -2.860652      55.51
 H       2.386244     0.487817    -3.970899      16.08
 C       2.184005     2.475725    -0.967913      46.33
 C       1.655358     3.732332    -0.340841      84.10
 H       2.028350     4.603034    -1.174771      17.52
 O       2.058188     4.163688     1.027403     259.36
 H       3.046364     4.310540     1.273117      28.02
 C       0.054024     3.871934    -0.322356      62.74
 H      -0.251085     3.400672    -1.277718      21.42
 C      -0.515552     5.349237     0.105694     112.11
 O      -0.088839     6.421444    -0.781450     282.35
 H      -0.327688     6.023018    -1.611861      30.95
 H      -0.007401     5.267859     1.018959      26.06
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 H      -1.543757     5.442433     0.338842      26.60
 C      -1.205388    -0.712819    -0.159048      25.15
 H      -0.568393    -1.671998     0.091380      17.49
 C      -3.196478     0.570066    -0.939471      60.88
 H      -4.146615     0.456501    -1.363121      18.27
 C      -2.504900     1.686629    -0.670396      10.91
 O      -3.054612     3.016743    -1.068835     149.15
 C      -4.638992     3.098596    -0.945805     113.46
 H      -4.688055     3.163777     0.058117      27.28
 H      -4.334782     3.849456    -1.780115      22.28
 H      -5.152248     2.360049    -1.554303      25.71
 C      -1.177784     1.675473    -0.099823       8.84
 O      -0.643815     2.786137     0.523308     170.81
 C      -0.489587     0.453491     0.157650      20.61
 H       0.323808     0.422623     0.997141      16.11
 C      -2.501947    -0.580521    -0.867855      26.71
 C      -3.244045    -1.934918    -1.228671      82.28
 H      -3.944961    -1.560415    -2.033244      21.91
 O      -2.417984    -2.695579    -2.064351     253.06
 H      -2.579501    -3.760527    -1.972181      19.38
 C      -3.988945    -2.642965    -0.085042     103.47
 H      -3.332300    -2.967694     0.699349      22.94
 O      -4.875150    -1.622189     0.563350     416.69
 H      -4.510514    -1.483176     1.340541      34.45
 C      -4.864174    -3.867551    -0.385416      87.93
 O      -4.027832    -5.049437    -0.973648     322.69
 H      -3.371381    -5.444520    -0.399357      29.24
 H      -5.646888    -3.617518    -1.049119      27.57
 H      -5.344275    -4.092748     0.542650      27.96
55
name = lig-etoh-frame_684
 C       1.814903     1.979723    -2.222107      90.24
 H       1.094147     2.490610    -2.953746      25.64
 C       3.153165     1.772601    -0.176363      39.48
 H       3.573619     1.990938     0.815635      21.98
 C       3.782847     0.574141    -0.742698      35.94
 O       4.422785    -0.269566     0.260160     242.70
 C       5.888647     0.094302     0.344453      89.00
 H       5.962255     1.030248     1.062167      24.62
 H       6.474775     0.561925    -0.616287      23.00
 H       6.257739    -0.734745     0.840167      26.48
 C       3.483003     0.232804    -2.025085      27.54
 O       4.252069    -0.866204    -2.743064     249.32
 H       4.652929    -1.235238    -2.046498      31.40
 C       2.622142     0.944028    -2.877514      39.33
 H       2.484276     0.574698    -3.897489      16.88
 C       2.226576     2.423103    -0.970884      30.17
 C       1.619614     3.802523    -0.364791      88.78
 H       2.094949     4.588819    -1.053101      18.83
 O       2.077422     4.117092     1.029333     290.32
 H       3.049443     4.327601     0.939660      27.05
 C      -0.031057     3.881425    -0.291719      79.05
 H      -0.216869     3.659062    -1.354775      21.05
 C      -0.508709     5.291399     0.041616      99.15
 O      -0.062228     6.417254    -0.731303     231.90
 H      -0.282567     6.124507    -1.698864      27.86
 H      -0.035000     5.526938     1.104600      22.87
 H      -1.672243     5.294058     0.281701      23.72
 C      -1.204529    -0.678566    -0.128118      40.36
 H      -0.785370    -1.701931    -0.217586      20.07
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 C      -3.225262     0.524085    -0.866745      42.90
 H      -4.266118     0.641297    -1.376521      17.30
 C      -2.417901     1.751905    -0.702265      18.63
 O      -2.996541     2.947879    -1.079680     143.66
 C      -4.600094     3.068756    -1.041301      81.95
 H      -4.707274     3.088402     0.217737      23.26
 H      -4.759351     4.177829    -1.511769      23.82
 H      -5.286946     2.264147    -1.395350      23.42
 C      -1.240337     1.628810    -0.088088      25.53
 O      -0.642585     2.794091     0.579451     162.68
 C      -0.482489     0.482864     0.142615      39.86
 H       0.482326     0.280829     0.716747      17.58
 C      -2.454090    -0.585765    -0.876307      24.08
 C      -3.235991    -1.882833    -1.192637      82.15
 H      -3.917274    -1.454725    -1.943482      23.18
 O      -2.366932    -2.700444    -2.048298     225.43
 H      -2.656359    -3.756499    -1.832884      17.56
 C      -3.969164    -2.615382    -0.105671      82.22
 H      -3.077127    -2.813727     0.608525      20.40
 O      -4.817130    -1.653103     0.568161     335.13
 H      -4.410730    -1.387574     1.657510      21.37
 C      -4.860795    -3.871921    -0.422255      69.27
 O      -4.020466    -5.002824    -0.975144     289.29
 H      -3.410585    -5.382364    -0.273434      26.18
 H      -5.641438    -3.855388    -1.272995      23.76
 H      -5.038888    -4.307237     0.736405      23.93
55
name = lig-etoh-frame_685
 C       1.845479     1.934641    -2.240390      65.27
 H       1.089326     2.471110    -2.723138      28.12
 C       3.121171     1.733921    -0.195674      52.92
 H       3.709004     2.167772     0.627284      23.22
 C       3.703080     0.609403    -0.666394      39.24
 O       4.451802    -0.219859     0.181434     270.90
 C       5.840490     0.103748     0.373023     107.61
 H       5.902950     0.785213     1.161529      26.79
 H       6.161628     0.439272    -0.573572      27.64
 H       6.241164    -0.844966     0.928966      24.66
 C       3.540284     0.237823    -2.067582      20.98
 O       4.237943    -0.876262    -2.816738     151.69
 H       4.853783    -1.351774    -2.031598      22.69
 C       2.593180     0.996118    -2.841689      49.00
 H       2.505601     0.689823    -3.925790      17.85
 C       2.223949     2.438562    -0.923180      53.49
 C       1.562766     3.840656    -0.340904      83.39
 H       2.011372     4.800119    -1.065866      18.22
 O       2.100888     4.064855     1.006699     284.96
 H       3.004040     4.262571     0.702785      28.00
 C      -0.067584     3.858702    -0.318823      80.78
 H      -0.397267     3.916757    -1.391787      21.16
 C      -0.513849     5.244791     0.077644     108.47
 O      -0.046448     6.391972    -0.706407     203.05
 H      -0.047936     6.414435    -1.729794      29.00
 H      -0.233053     5.717924     0.964301      24.72
 H      -1.566319     5.137709     0.002019      26.28
 C      -1.216146    -0.674637    -0.172605      71.33
 H      -0.856285    -1.702294    -0.307531      21.90
 C      -3.223101     0.566697    -0.841236      38.16
 H      -4.161645     0.665526    -1.239979      18.76
 C      -2.450348     1.774546    -0.752474      13.41
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 O      -2.969413     2.897175    -1.098935     197.91
 C      -4.522650     3.069745    -1.066635     109.01
 H      -4.839163     3.106348    -0.123084      28.83
 H      -5.102581     4.151587    -1.235900      24.01
 H      -5.172617     2.246724    -1.370324      24.94
 C      -1.194917     1.669955    -0.015213      10.56
 O      -0.632286     2.832507     0.615623     172.31
 C      -0.500375     0.457162     0.140622      52.89
 H       0.555777     0.468776     0.418514      20.74
 C      -2.415608    -0.680977    -0.806788      25.97
 C      -3.226494    -1.799489    -1.245926      77.88
 H      -4.180871    -1.451993    -1.807952      23.76
 O      -2.314063    -2.740813    -2.014856     262.81
 H      -2.664644    -3.543635    -1.815593      25.29
 C      -3.931724    -2.570486    -0.075831      78.63
 H      -3.077037    -2.960110     0.460266      24.33
 O      -4.753275    -1.670917     0.599398     397.26
 H      -4.589312    -1.561904     1.565306      30.14
 C      -4.795156    -3.920981    -0.428795     101.70
 O      -3.999957    -4.951914    -0.986832     331.26
 H      -3.560296    -5.315414    -0.116020      26.34
 H      -5.600592    -3.844856    -1.113027      27.27
 H      -5.147894    -4.261121     0.460157      29.35
55
name = lig-etoh-frame_686
 C       1.863786     1.962693    -2.210182       9.41
 H       0.980288     2.508621    -2.685442      20.12
 C       3.122027     1.736776    -0.172860      42.18
 H       3.571058     2.311104     0.624127      19.06
 C       3.655693     0.565823    -0.658396      27.32
 O       4.463638    -0.188444     0.100687     271.79
 C       5.777858     0.082146     0.437728     105.75
 H       5.930804     0.902415     1.297049      25.81
 H       6.250408     0.347439    -0.602853      26.85
 H       6.344036    -0.819380     0.617282      26.65
 C       3.609782     0.213925    -2.128237      34.12
 O       4.194879    -0.851936    -2.825497     148.62
 H       5.032508    -1.412098    -2.371339      20.07
 C       2.606931     0.976630    -2.818389      55.58
 H       2.444036     0.856592    -3.988221      24.59
 C       2.147478     2.509580    -0.904324      53.37
 C       1.515004     3.829147    -0.329246     109.98
 H       1.615967     4.765215    -0.941693      21.12
 O       2.113427     4.017100     0.961906     253.03
 H       3.138661     4.224242     0.843876      26.25
 C      -0.030566     3.848942    -0.358935      81.79
 H      -0.584395     3.753726    -1.305407      20.93
 C      -0.547175     5.239594     0.115628      91.11
 O      -0.018024     6.384444    -0.692366     222.53
 H       0.018096     6.269024    -1.644463      30.59
 H      -0.417901     5.608077     1.215856      23.16
 H      -1.668534     5.131691    -0.229662      23.27
 C      -1.196531    -0.743430    -0.256159      54.00
 H      -0.543643    -1.726487    -0.167733      21.44
 C      -3.132569     0.595322    -0.841585      59.21
 H      -4.229147     0.524517    -1.191241      19.68
 C      -2.489527     1.699457    -0.738734      11.72
 O      -3.005535     2.948037    -1.142592     222.14
 C      -4.437271     3.073953    -1.065545     105.34
 H      -4.848238     2.960434     0.158424      23.52
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 H      -5.034150     4.024732    -1.390077      24.87
 H      -4.864554     2.254858    -1.688398      24.08
 C      -1.133492     1.749290     0.059206      -9.98
 O      -0.616916     2.885196     0.616889     183.96
 C      -0.527202     0.455835     0.152765      29.29
 H       0.643619     0.692592     0.190670      19.36
 C      -2.488673    -0.682714    -0.718454      35.90
 C      -3.245236    -1.784921    -1.327405      79.80
 H      -4.113207    -1.497300    -1.868265      25.46
 O      -2.274471    -2.752059    -1.972280     164.80
 H      -2.835367    -3.787050    -1.818097      15.13
 C      -3.883703    -2.569639    -0.046394      77.77
 H      -3.080856    -3.131766     0.562938      22.17
 O      -4.715016    -1.678848     0.622993     329.55
 H      -4.563690    -1.718125     1.713778      24.25
 C      -4.715771    -3.919948    -0.439044      75.21
 O      -3.950328    -4.923847    -0.989653     308.91
 H      -3.567985    -5.433189    -0.290236      28.87
 H      -5.644143    -3.555105    -1.055462      25.88
 H      -5.530911    -4.213485     0.521393      26.14
55
name = lig-etoh-frame_687
 C       1.844786     2.056964    -2.151164      22.44
 H       1.086519     2.393468    -2.834970      19.80
 C       3.094404     1.807944    -0.159027      45.83
 H       3.411990     2.158551     0.862058      17.38
 C       3.645937     0.508103    -0.744594      23.46
 O       4.456891    -0.215677     0.059464     287.64
 C       5.770566     0.093053     0.464424     119.64
 H       5.922038     0.833839     1.154860      30.59
 H       6.465554     0.518949    -0.310027      29.09
 H       6.326489    -0.897751     0.536239      26.03
 C       3.636268     0.211039    -2.145180      31.97
 O       4.157815    -0.831042    -2.825546     243.17
 H       4.927190    -1.194423    -2.541591      24.12
 C       2.639668     0.933254    -2.830002      37.62
 H       2.444170     0.844972    -3.822613      29.75
 C       2.084087     2.550187    -0.910836      45.33
 C       1.480297     3.762948    -0.334298     104.30
 H       1.596898     4.854567    -1.095816      18.05
 O       2.119286     3.987797     0.932366     282.26
 H       3.040537     4.180711     1.007590      30.27
 C       0.005422     3.860783    -0.349702      78.37
 H      -0.438918     3.447214    -1.287255      20.24
 C      -0.619601     5.268454     0.119560     106.07
 O       0.018861     6.380492    -0.654943     212.51
 H      -0.078699     5.878395    -1.605214      26.37
 H      -0.592853     5.232751     1.193444      25.18
 H      -1.626646     5.272371    -0.126866      25.49
 C      -1.118672    -0.813435    -0.318584      25.28
 H      -0.483180    -1.597149    -0.152721      22.06
 C      -3.102216     0.523743    -0.874058      61.54
 H      -4.131999     0.456787    -1.153517      22.85
 C      -2.430758     1.746421    -0.645382      -4.32
 O      -3.038732     3.034218    -1.181497     195.04
 C      -4.393569     3.031185    -1.023855     116.66
 H      -4.617755     2.751781    -0.109564      27.47
 H      -4.673546     4.137279    -1.628784      22.80
 H      -4.672820     2.368195    -1.874633      23.61
 C      -1.148097     1.772462     0.080951       6.87
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 O      -0.597327     2.938253     0.608530     186.22
 C      -0.533020     0.508563     0.150463      21.41
 H       0.487586     0.511186     0.260479      20.62
 C      -2.565659    -0.658860    -0.653258      13.58
 C      -3.251319    -1.867929    -1.342340      66.29
 H      -4.001969    -1.507611    -2.206047      21.34
 O      -2.278002    -2.778472    -1.923567     254.31
 H      -2.662153    -3.588802    -1.966407      22.97
 C      -3.836318    -2.638563    -0.030537      89.93
 H      -3.033423    -2.914215     0.654752      22.09
 O      -4.688845    -1.672568     0.666761     300.21
 H      -4.485448    -1.857621     1.750122      23.23
 C      -4.736187    -3.838264    -0.404683      92.47
 O      -3.891688    -4.919522    -1.011180     328.96
 H      -3.444444    -5.630188    -0.420145      26.16
 H      -5.319352    -3.408049    -1.212224      27.39
 H      -5.282732    -4.154217     0.353074      29.16
55
name = lig-etoh-frame_688
 C       1.852732     2.075355    -2.195524      40.24
 H       1.158507     2.457515    -2.961985      18.46
 C       3.063761     1.828425    -0.184878      76.92
 H       3.202062     1.791434     0.891773      18.66
 C       3.653660     0.553286    -0.806595      29.41
 O       4.448350    -0.284461     0.042937     258.88
 C       5.823145     0.098660     0.443356      91.55
 H       5.787781     0.812070     1.436523      26.44
 H       6.463332     0.727017    -0.273549      27.75
 H       6.170897    -0.890512     0.810235      25.71
 C       3.597075     0.240115    -2.143322      22.08
 O       4.112028    -0.827311    -2.842540     115.97
 H       5.188981    -1.053212    -2.401242      18.96
 C       2.630169     0.970939    -2.787278      52.31
 H       2.399072     0.649612    -3.985252      24.59
 C       2.083227     2.540473    -0.891580      56.70
 C       1.499327     3.770400    -0.363050     121.47
 H       1.868791     4.455411    -1.055041      23.94
 O       2.081494     3.975117     0.937536     267.07
 H       3.083243     4.201940     0.869769      29.62
 C      -0.018350     3.872585    -0.317791      85.19
 H      -0.102653     3.478023    -1.356416      21.03
 C      -0.668218     5.273801     0.089787      95.29
 O       0.042117     6.344986    -0.614033     241.99
 H      -0.076032     5.969849    -1.510668      29.99
 H      -0.534363     5.159373     1.211361      23.93
 H      -1.836729     5.356311    -0.091964      23.15
 C      -1.084475    -0.749464    -0.341501      19.47
 H      -0.442179    -1.791338    -0.231146      18.24
 C      -3.105187     0.527387    -0.905786      30.94
 H      -4.152004     0.556657    -1.268024      22.54
 C      -2.375853     1.858121    -0.550714      -4.47
 O      -2.972654     3.082634    -1.181720     178.23
 C      -4.390996     3.014708    -1.091938     104.08
 H      -4.792422     2.585023     0.018793      23.70
 H      -4.408637     4.109270    -1.345289      24.00
 H      -4.911719     2.375672    -1.843987      24.91
 C      -1.208955     1.778452     0.069568      27.60
 O      -0.586144     2.965401     0.617635     203.49
 C      -0.546359     0.504153     0.118848      23.31
 H       0.554957     0.286129     0.605980      18.06
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 C      -2.521434    -0.748331    -0.636242      -2.21
 C      -3.253427    -1.976758    -1.299684      84.79
 H      -3.812467    -1.667997    -2.122409      21.68
 O      -2.260787    -2.774481    -1.888295     218.72
 H      -2.706224    -3.789700    -2.042937      14.67
 C      -3.817824    -2.682960    -0.022950      97.03
 H      -2.886225    -2.751953     0.602475      19.94
 O      -4.660787    -1.677521     0.720161     356.58
 H      -4.491796    -1.729755     1.628143      28.72
 C      -4.706119    -3.752338    -0.406164      67.52
 O      -3.841752    -4.918981    -1.052814     271.97
 H      -3.426913    -5.564441    -0.358970      24.32
 H      -5.183753    -3.472169    -1.380027      24.63
 H      -5.307382    -4.298086     0.577942      23.40
55
name = lig-etoh-frame_689
 C       1.883966     2.047026    -2.306653      53.28
 H       1.202870     2.692731    -2.911239      19.32
 C       3.053072     1.740095    -0.229245      80.40
 H       3.007528     1.630262     0.875547      18.40
 C       3.699646     0.657451    -0.784935      47.50
 O       4.443378    -0.347694     0.019363     231.88
 C       5.850366     0.122894     0.479489     100.17
 H       5.607589     0.571184     1.359144      28.53
 H       6.340148     0.733061    -0.357145      26.70
 H       6.260276    -0.780200     0.915570      26.97
 C       3.527024     0.269645    -2.145065      12.55
 O       4.112780    -0.834694    -2.841582     212.52
 H       4.908230    -0.980916    -2.391767      26.21
 C       2.557410     1.049059    -2.805621      31.78
 H       2.413674     0.657622    -3.671806      24.77
 C       2.107140     2.476796    -0.897620      87.53
 C       1.545850     3.796071    -0.337252      97.32
 H       2.150828     4.598390    -1.233736      19.25
 O       2.041952     3.985884     0.966030     268.46
 H       3.004066     4.194457     0.733451      29.45
 C      -0.055079     3.886781    -0.321241      87.14
 H      -0.210660     3.727391    -1.406120      20.84
 C      -0.703560     5.248309     0.060697     111.04
 O       0.049925     6.300778    -0.566870     227.86
 H       0.040789     6.287736    -1.593735      29.17
 H      -0.397257     5.478258     1.104151      25.41
 H      -1.733398     5.303848    -0.102182      27.05
 C      -1.085070    -0.677203    -0.333475      63.20
 H      -0.636440    -1.554568    -0.366656      22.01
 C      -3.071533     0.582899    -0.900220      13.10
 H      -4.077652     0.689613    -1.426925      20.64
 C      -2.448376     1.910521    -0.553166       0.45
 O      -2.857662     3.069974    -1.139425     181.20
 C      -4.417418     3.001597    -1.133526      99.86
 H      -4.836951     2.799814    -0.251519      28.08
 H      -4.755585     4.296311    -1.097443      23.19
 H      -5.059967     2.448345    -1.836384      24.69
 C      -1.187919     1.790399     0.089732       4.89
 O      -0.588772     2.950168     0.636343     202.88
 C      -0.517065     0.453566     0.112236      43.90
 H       0.251027     0.431654     0.756241      19.12
 C      -2.440890    -0.804941    -0.697763      -5.10
 C      -3.210720    -2.047751    -1.197306      76.00
 H      -4.076745    -1.708357    -1.973116      19.96
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 O      -2.219178    -2.809784    -1.874850     226.44
 H      -2.660718    -3.783395    -1.978826      15.23
 C      -3.802018    -2.641602     0.012682      98.50
 H      -2.854775    -2.983251     0.520150      20.65
 O      -4.641803    -1.694095     0.726858     324.04
 H      -4.341670    -1.529220     1.904927      19.57
 C      -4.666198    -3.789346    -0.407690      97.37
 O      -3.805060    -4.910706    -1.088917     327.97
 H      -3.433207    -5.309091    -0.308725      29.10
 H      -5.388997    -3.569504    -1.231871      26.95
 H      -5.255787    -4.118711     0.286108      28.75
55
name = lig-etoh-frame_690
 C       1.868983     2.136042    -2.334997      25.91
 H       1.252663     2.797554    -2.881461      23.89
 C       3.026450     1.624845    -0.213044      79.01
 H       2.966161     1.765600     0.857874      18.91
 C       3.802769     0.671238    -0.776857      60.87
 O       4.451126    -0.383908    -0.016874     238.81
 C       5.810261     0.119637     0.515515      90.38
 H       5.506758     0.818947     1.448124      23.33
 H       6.305182     0.643451    -0.272444      24.96
 H       6.585775    -0.749028     0.704586      24.58
 C       3.461120     0.300525    -2.126897      49.02
 O       4.086862    -0.813486    -2.827364     165.25
 H       4.922299    -1.141060    -2.231300      26.32
 C       2.530902     1.042394    -2.870976      70.54
 H       2.242026     0.609990    -4.015218      16.56
 C       2.115578     2.412968    -0.975691      37.72
 C       1.592912     3.825751    -0.340541     100.72
 H       1.921088     4.594454    -0.906026      21.64
 O       2.009790     4.015366     0.995863     311.39
 H       2.982921     4.188043     1.026783      28.31
 C      -0.062693     3.919495    -0.358115      71.81
 H      -0.618770     3.807257    -1.337952      20.63
 C      -0.666511     5.232274     0.049176     101.47
 O       0.057703     6.279929    -0.548058     217.86
 H       0.061061     6.514430    -1.568466      27.57
 H      -0.492392     5.635947     1.059094      24.20
 H      -1.821836     5.201865    -0.175162      24.19
 C      -1.136101    -0.667126    -0.334238      40.13
 H      -0.442335    -1.677902    -0.390426      18.12
 C      -3.017525     0.623947    -0.887733      54.93
 H      -3.885541     0.653952    -1.471126      21.03
 C      -2.503416     1.837800    -0.585357       5.57
 O      -2.813293     3.054657    -1.089864     172.44
 C      -4.436898     3.099788    -1.179741      90.74
 H      -4.793764     2.723967    -0.034451      23.53
 H      -5.032542     3.960957    -1.071991      26.26
 H      -4.873734     2.562784    -2.059300      24.32
 C      -1.147463     1.770263     0.107208      -3.99
 O      -0.592534     2.908880     0.650329     184.49
 C      -0.506033     0.516716     0.146358      29.23
 H       0.391789     0.567247     0.933884      16.25
 C      -2.408278    -0.715096    -0.814232      26.74
 C      -3.146526    -2.019659    -1.134108      92.08
 H      -4.069280    -1.802853    -1.587657      23.39
 O      -2.174689    -2.870486    -1.869376     257.97
 H      -2.569577    -3.759083    -1.888793      18.02
 C      -3.788178    -2.619974     0.086957      85.33
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 H      -3.020756    -3.249354     0.662846      20.51
 O      -4.614030    -1.704386     0.757522     410.92
 H      -4.257845    -1.594902     1.623823      31.08
 C      -4.626358    -3.870189    -0.470175      76.54
 O      -3.795229    -4.880698    -1.107491     320.76
 H      -3.240317    -5.255646    -0.264550      24.79
 H      -5.486274    -3.512050    -1.074717      26.76
 H      -5.409387    -4.265809     0.493871      25.60
55
name = lig-etoh-frame_691
 C       1.854708     2.244920    -2.335141      66.18
 H       1.195459     2.897102    -2.993141      23.85
 C       2.963949     1.559385    -0.165600      61.07
 H       3.083918     1.953608     0.878066      19.87
 C       3.892075     0.594604    -0.800341      39.95
 O       4.494052    -0.399728    -0.052199     279.26
 C       5.743667     0.105155     0.559040     111.01
 H       5.696156     0.857002     1.278220      26.75
 H       6.289929     0.785870    -0.269265      24.60
 H       6.487915    -0.610602     0.615783      27.21
 C       3.433080     0.303516    -2.136174      14.23
 O       4.061032    -0.765068    -2.789841     163.98
 H       4.670934    -1.414157    -2.095033      23.20
 C       2.507557     0.984685    -2.995243      19.09
 H       2.244419     0.759906    -3.929078      19.59
 C       2.125633     2.405376    -1.030281      26.89
 C       1.578487     3.789371    -0.341655      75.06
 H       1.889872     4.925377    -0.998789      18.86
 O       1.972285     4.045967     1.040312     294.34
 H       2.949820     4.203143     1.324221      26.12
 C      -0.054656     3.923847    -0.382911      64.53
 H      -0.653482     3.633605    -1.233525      20.67
 C      -0.638011     5.249731     0.062533     109.33
 O       0.081865     6.314960    -0.562428     262.67
 H      -0.124521     6.288260    -1.480236      31.34
 H      -0.730562     5.397519     1.192238      24.87
 H      -1.658179     5.164638    -0.241812      25.74
 C      -1.115764    -0.707096    -0.322858       6.65
 H      -0.491950    -1.505066    -0.277840      19.85
 C      -3.012721     0.601028    -0.919870      68.21
 H      -3.975291     0.556980    -1.580011      17.35
 C      -2.425124     1.749474    -0.580566       9.24
 O      -2.856670     3.068060    -1.047105     155.72
 C      -4.441694     3.157197    -1.165017      93.60
 H      -4.590062     2.476880    -0.425122      25.37
 H      -5.048751     4.321067    -1.229099      22.85
 H      -4.526244     2.628108    -2.119224      24.04
 C      -1.158580     1.745780     0.092946      21.40
 O      -0.588820     2.875651     0.656706     159.22
 C      -0.490420     0.605141     0.231458      20.00
 H       0.456140     0.512160     0.682718      19.23
 C      -2.393236    -0.577131    -0.922507      32.89
 C      -3.046939    -1.949248    -1.091147      59.53
 H      -4.071545    -1.774106    -1.692651      22.67
 O      -2.139372    -2.906081    -1.859233     179.41
 H      -2.642295    -3.964890    -1.761616      10.56
 C      -3.765953    -2.692707     0.163635      70.94
 H      -3.208663    -3.198206     1.000340      21.02
 O      -4.600677    -1.717524     0.743332     344.78
 H      -4.152000    -1.637183     1.858996      19.62
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 C      -4.651431    -3.941666    -0.470683      95.62
 O      -3.790522    -4.849619    -1.102110     365.43
 H      -3.185947    -5.336372    -0.544811      28.93
 H      -5.387007    -3.464333    -1.189249      27.51
 H      -4.988529    -4.393361     0.334160      29.34
55
name = lig-etoh-frame_692
 C       1.877744     2.250576    -2.420976      28.51
 H       1.249109     2.921088    -2.961153      21.29
 C       2.931525     1.525201    -0.157771      67.94
 H       3.214019     1.966148     0.789852      23.17
 C       3.842807     0.557041    -0.811432      34.67
 O       4.565419    -0.414642    -0.076518     262.36
 C       5.706995     0.132538     0.523755     103.01
 H       5.661336     0.832485     1.480591      24.53
 H       6.126102     0.773715    -0.183995      26.43
 H       6.389502    -0.823183     0.810005      24.42
 C       3.433279     0.277542    -2.190033      19.91
 O       4.041326    -0.749697    -2.747626     238.36
 H       4.329660    -1.288055    -2.140830      30.43
 C       2.470206     1.020026    -3.006750      26.91
 H       2.292463     0.644623    -4.111258      20.80
 C       2.147880     2.464228    -0.984220      27.81
 C       1.552843     3.787675    -0.365211      99.16
 H       1.841935     4.556093    -0.933812      23.78
 O       1.912032     4.064845     1.095115     311.68
 H       2.893270     4.240145     1.138418      27.13
 C      -0.025616     3.872829    -0.354808      56.25
 H      -0.331566     3.464295    -1.374013      19.38
 C      -0.618476     5.265472     0.100458      96.29
 O       0.096472     6.366072    -0.580267     224.69
 H      -0.222970     6.060157    -1.533562      25.91
 H      -0.715864     5.157681     1.159134      24.74
 H      -1.678190     5.273276    -0.372843      22.13
 C      -1.055669    -0.627645    -0.280664      12.06
 H      -0.494972    -1.681323    -0.175302      19.00
 C      -3.102304     0.581282    -1.025599      44.29
 H      -4.018720     0.595816    -1.480821      18.61
 C      -2.333396     1.766993    -0.584554       2.92
 O      -2.923463     3.085781    -0.988438     166.36
 C      -4.401769     3.200834    -1.177414     110.60
 H      -4.876611     2.283977    -0.546934      21.74
 H      -4.529198     4.264546    -1.252277      25.22
 H      -4.438469     2.788387    -2.219700      23.91
 C      -1.181271     1.775133     0.085310      24.84
 O      -0.581629     2.870139     0.656603     167.27
 C      -0.488335     0.540238     0.282484      32.58
 H       0.622041     0.523500     0.531647      20.05
 C      -2.307168    -0.574473    -0.963918      23.04
 C      -2.984349    -1.919670    -1.094509      75.19
 H      -3.735119    -1.752337    -1.809215      23.72
 O      -2.124166    -2.936525    -1.830377     264.22
 H      -2.616887    -3.647863    -1.727201      22.69
 C      -3.747777    -2.779832     0.212247      66.16
 H      -3.114182    -3.064323     1.075007      20.68
 O      -4.586714    -1.723736     0.758715     363.04
 H      -4.517377    -1.657781     1.698044      29.06
 C      -4.641083    -3.941725    -0.439391      81.11
 O      -3.772262    -4.841325    -1.146530     348.41
 H      -3.258102    -5.474828    -0.534222      25.45
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 H      -5.278288    -3.617393    -1.247443      26.49
 H      -5.024940    -4.669765     0.525506      23.85
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name = lig-etoh-frame_693
 C       1.942309     2.192215    -2.468285      49.76
 H       1.308631     2.933454    -3.007749      17.98
 C       2.938354     1.539573    -0.201488      52.66
 H       3.254236     1.822763     0.828882      21.44
 C       3.675905     0.551964    -0.825474      21.81
 O       4.603847    -0.427168    -0.115467     248.21
 C       5.727444     0.153360     0.530294     106.57
 H       5.344746     0.518678     1.475621      26.01
 H       6.311234     0.860291    -0.262825      24.57
 H       6.182480    -0.683811     0.884660      27.29
 C       3.416885     0.294773    -2.212468      25.75
 O       4.029815    -0.769609    -2.765622     131.56
 H       4.278082    -1.440759    -1.828921      18.32
 C       2.445455     1.091564    -2.972216      39.09
 H       2.433981     0.543199    -3.948974      24.48
 C       2.170451     2.513864    -0.939305      65.97
 C       1.509251     3.744659    -0.317778      85.82
 H       2.003487     4.692097    -1.171546      18.96
 O       1.856311     4.075155     1.117130     294.68
 H       2.795877     4.302207     0.964870      26.53
 C       0.012824     3.793794    -0.323625      80.57
 H      -0.082425     3.542366    -1.368893      19.36
 C      -0.615122     5.245671     0.085585      91.95
 O       0.084742     6.392321    -0.594337     212.56
 H       0.063549     6.214807    -1.616320      27.14
 H      -0.511884     5.254825     1.236035      23.21
 H      -1.629706     5.381606    -0.289752      24.02
 C      -0.978455    -0.560562    -0.239030      65.88
 H      -0.687360    -1.585544    -0.126311      20.21
 C      -3.104418     0.594114    -1.117679      18.82
 H      -4.239574     0.670782    -1.443322      19.22
 C      -2.391333     1.827505    -0.663328      -4.44
 O      -2.968402     3.089559    -0.896320     194.78
 C      -4.302421     3.143203    -1.218242     120.38
 H      -5.247458     2.815501    -0.699139      24.66
 H      -4.379118     4.435270    -1.073349      22.79
 H      -4.619860     3.040812    -2.276987      24.96
 C      -1.140588     1.779663     0.115694      -4.10
 O      -0.567612     2.895507     0.646630     189.76
 C      -0.470075     0.454755     0.308276      52.26
 H       0.598807     0.627855     0.545435      20.17
 C      -2.230967    -0.635921    -0.938989      -2.93
 C      -2.926639    -1.961918    -1.126399      60.84
 H      -3.759861    -1.720816    -1.940153      19.57
 O      -2.083960    -2.913058    -1.788936     183.37
 H      -2.812129    -3.855810    -1.759394      10.79
 C      -3.749838    -2.791421     0.228764      63.68
 H      -2.805392    -3.071692     0.862880      21.15
 O      -4.589735    -1.732031     0.734015     276.53
 H      -4.835643    -1.777323     1.855749      24.40
 C      -4.588873    -3.962497    -0.336498     102.87
 O      -3.737487    -4.861711    -1.212468     328.01
 H      -3.442089    -5.508690    -0.451784      24.62
 H      -5.391563    -3.660933    -1.092555      27.21
 H      -5.249300    -4.450472     0.272412      28.70
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name = lig-etoh-frame_694
 C       1.975007     2.225311    -2.394523      27.85
 H       1.399189     2.847245    -3.099489      14.69
 C       2.955139     1.623279    -0.226784      59.65
 H       3.123024     1.627884     0.854727      18.39
 C       3.521266     0.507911    -0.853584      24.01
 O       4.581461    -0.424307    -0.198220     237.16
 C       5.741460     0.187043     0.536392      95.06
 H       5.171880     0.609030     1.420227      26.96
 H       6.426711     0.789164     0.060689      28.95
 H       6.409219    -0.762717     0.892318      26.22
 C       3.385353     0.328053    -2.186946      29.72
 O       4.022722    -0.835603    -2.778622     201.26
 H       4.389199    -1.269977    -1.992324      19.23
 C       2.508855     1.060558    -2.946871      44.24
 H       2.334378     0.731079    -3.964331      27.35
 C       2.189079     2.509184    -0.948944      72.25
 C       1.517597     3.749484    -0.261398     126.04
 H       1.778879     4.479999    -0.844604      25.58
 O       1.822237     4.076984     1.093476     277.80
 H       2.812094     4.416569     1.147139      27.75
 C       0.036416     3.770506    -0.316089      83.73
 H      -0.319347     3.575674    -1.383207      20.78
 C      -0.574631     5.220174     0.043360      92.68
 O       0.071065     6.400591    -0.607286     235.91
 H       0.290023     6.373442    -1.534159      30.18
 H      -0.334036     5.547231     1.033904      24.26
 H      -1.705349     5.270682    -0.100674      24.57
 C      -0.994330    -0.643052    -0.265894      43.18
 H      -0.517431    -1.642143    -0.044626      20.00
 C      -3.011291     0.607723    -1.171758      57.02
 H      -4.040414     0.587292    -1.378106      24.94
 C      -2.467674     1.838850    -0.737929      -3.90
 O      -2.981025     3.066088    -0.780549     203.03
 C      -4.278765     3.200977    -1.289516     144.33
 H      -5.197938     3.095100    -0.606726      25.06
 H      -4.447952     4.197131    -0.956313      26.21
 H      -4.593278     3.179274    -2.342111      26.42
 C      -1.124967     1.722920     0.119523     -14.07
 O      -0.553902     2.923561     0.636556     193.36
 C      -0.408835     0.565605     0.358580      47.54
 H       0.571588     0.570082     0.801146      19.83
 C      -2.238921    -0.647087    -0.883511       9.84
 C      -2.921466    -2.027121    -1.191925      82.69
 H      -3.786361    -1.772244    -1.739944      21.83
 O      -2.052830    -2.919281    -1.741542     283.10
 H      -2.422710    -3.719099    -1.880961      21.46
 C      -3.720128    -2.736731     0.204708      85.56
 H      -2.827172    -3.108297     0.676715      23.33
 O      -4.613182    -1.750536     0.714370     346.28
 H      -4.722332    -1.967403     1.596817      28.09
 C      -4.544361    -3.958937    -0.295633      85.54
 O      -3.726743    -4.894125    -1.241219     332.93
 H      -3.319030    -5.515763    -0.637093      28.87
 H      -5.311777    -3.443808    -0.867125      28.32
 H      -5.397240    -4.501838     0.441125      27.22
55
name = lig-etoh-frame_695
 C       1.997432     2.277770    -2.285559      34.91
 H       1.433214     2.843040    -2.995363      19.40
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 C       2.988909     1.678104    -0.215365      87.26
 H       2.932219     1.672873     0.878246      20.95
 C       3.451936     0.456231    -0.822066      25.25
 O       4.535727    -0.401888    -0.303333     216.95
 C       5.718453     0.166382     0.576896      97.93
 H       5.334819     0.865398     1.368469      27.20
 H       6.518838     0.975235     0.131000      25.68
 H       6.351082    -0.596016     0.812011      28.18
 C       3.383504     0.257300    -2.201713      26.31
 O       3.998642    -0.872150    -2.795885     179.38
 H       4.662633    -1.249320    -2.037191      18.22
 C       2.572056     1.039832    -2.943423      42.37
 H       2.190715     1.038809    -4.047495      23.80
 C       2.179057     2.518327    -0.981968      52.77
 C       1.540543     3.728543    -0.208787     103.95
 H       1.813803     4.877352    -0.948550      18.41
 O       1.825882     4.077359     1.080616     300.07
 H       2.676371     4.391750     1.347828      30.44
 C       0.005341     3.809273    -0.347578      86.25
 H      -0.519746     3.542989    -1.245434      21.95
 C      -0.512325     5.221839    -0.013520      98.69
 O       0.050455     6.404373    -0.620363     200.82
 H       0.364493     6.297948    -1.663221      25.16
 H      -0.231600     5.593368     1.023753      22.71
 H      -1.624665     5.044934     0.057911      24.62
 C      -1.006989    -0.736014    -0.267541      13.16
 H      -0.306451    -1.593179    -0.015680      19.31
 C      -2.876103     0.599474    -1.187738      77.15
 H      -3.958299     0.432789    -1.512453      24.48
 C      -2.441360     1.772024    -0.743184      14.45
 O      -2.987766     3.042101    -0.671836     161.12
 C      -4.333032     3.326660    -1.325681      96.35
 H      -4.907033     2.673957    -0.574945      22.83
 H      -4.482041     4.596313    -1.107678      22.62
 H      -4.309662     3.075539    -2.404435      24.42
 C      -1.146406     1.709871     0.087058       0.28
 O      -0.567239     2.925134     0.640283     155.91
 C      -0.379377     0.654148     0.363437      14.40
 H       0.466671     0.500752     1.132171      18.90
 C      -2.283014    -0.654277    -0.834303      12.92
 C      -2.976599    -2.059488    -1.196361      65.27
 H      -3.957699    -1.858204    -1.837775      19.75
 O      -1.969461    -2.916326    -1.714010     219.22
 H      -2.353625    -3.901770    -1.991980      12.79
 C      -3.657980    -2.678748     0.116460      85.35
 H      -2.847358    -3.038623     0.932631      18.82
 O      -4.629134    -1.778746     0.669865     304.88
 H      -4.590863    -2.006521     1.705346      24.20
 C      -4.532086    -3.955642    -0.287456      80.48
 O      -3.757768    -4.908084    -1.246052     334.65
 H      -3.071931    -5.530306    -0.714676      24.27
 H      -5.207993    -3.315021    -0.931739      27.23
 H      -4.865251    -4.502876     0.542268      29.19
55
name = lig-etoh-frame_696
 C       2.031084     2.257152    -2.269158      17.38
 H       1.354111     3.014832    -2.821705      20.05
 C       3.022245     1.658032    -0.188510      85.68
 H       2.903010     1.893762     0.892241      19.53
 C       3.468305     0.441295    -0.754907      29.17
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 O       4.508869    -0.366508    -0.374276     192.32
 C       5.673923     0.209491     0.579392      91.83
 H       5.399465     0.816244     1.439568      27.84
 H       6.184762     0.850328    -0.058085      28.08
 H       6.259169    -0.776261     0.919981      25.45
 C       3.384486     0.124159    -2.245022       2.82
 O       3.969459    -0.907021    -2.795590     123.86
 H       4.981704    -1.102010    -2.319994      19.96
 C       2.564589     1.129550    -2.945540      45.10
 H       2.373408     1.033670    -3.936720      25.83
 C       2.172099     2.571720    -0.926438      58.00
 C       1.570803     3.790302    -0.282542     113.67
 H       1.843893     4.542716    -0.759482      26.07
 O       1.827779     4.061537     1.113648     301.79
 H       2.807505     4.334588     1.279253      27.65
 C      -0.030469     3.861547    -0.372926      65.06
 H      -0.416025     3.495903    -1.371808      22.83
 C      -0.453098     5.244085    -0.002279     115.05
 O       0.029261     6.402571    -0.684269     294.73
 H       0.114921     6.151427    -1.582499      30.86
 H      -0.224673     5.249689     1.057303      24.68
 H      -1.553605     5.112533    -0.055098      24.59
 C      -0.974072    -0.732286    -0.206425      24.71
 H      -0.403742    -1.614954    -0.090071      20.31
 C      -2.817049     0.527183    -1.205586      62.14
 H      -3.759019     0.443385    -1.787383      25.83
 C      -2.332455     1.748669    -0.674824      15.10
 O      -2.996484     3.033402    -0.587479     133.66
 C      -4.359424     3.440845    -1.301081     124.14
 H      -4.886465     2.543959    -0.957066      23.71
 H      -4.497631     4.501350    -1.469402      25.39
 H      -4.085287     2.979243    -2.265110      25.36
 C      -1.163324     1.777971     0.050680      11.30
 O      -0.613580     2.915393     0.656779     156.60
 C      -0.409727     0.581056     0.322160      15.84
 H       0.253390     0.617304     1.118306      20.57
 C      -2.291128    -0.718721    -0.805099       0.23
 C      -3.056031    -2.054185    -1.167301      81.77
 H      -3.750923    -1.990100    -1.972112      20.16
 O      -1.875868    -2.924285    -1.704179     215.17
 H      -2.484033    -3.759464    -1.956276      14.29
 C      -3.580890    -2.665690     0.047036     112.97
 H      -2.974979    -2.767865     0.892555      19.58
 O      -4.646613    -1.814640     0.630038     333.93
 H      -4.380928    -1.669992     1.698300      23.80
 C      -4.452202    -3.929271    -0.330559      85.60
 O      -3.805424    -4.912235    -1.246065     360.14
 H      -3.150029    -5.308539    -0.631480      26.35
 H      -5.326542    -3.649565    -0.954234      26.36
 H      -4.559525    -4.524805     0.694162      25.44
55
name = lig-etoh-frame_697
 C       2.028998     2.263338    -2.284460      46.03
 H       1.445639     2.968094    -2.760335      23.91
 C       3.012836     1.641206    -0.145751      56.77
 H       3.209071     1.945881     0.890369      20.12
 C       3.525352     0.444838    -0.768506      13.74
 O       4.525870    -0.342810    -0.366810     189.74
 C       5.601464     0.219437     0.554138      97.89
 H       5.231577     0.681267     1.537680      25.90
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 H       6.080150     0.764851    -0.353387      24.07
 H       6.027105    -0.700937     0.881663      27.36
 C       3.303142     0.113868    -2.230179       9.21
 O       3.979642    -0.966492    -2.816231     201.18
 H       4.820090    -1.036072    -2.547229      29.24
 C       2.579867     1.184868    -2.920547      50.77
 H       2.566575     0.963019    -4.080621      20.12
 C       2.211050     2.571143    -0.843463      27.10
 C       1.553619     3.823532    -0.336248      82.66
 H       2.133996     4.862637    -1.060547      18.78
 O       1.851422     4.039097     1.157295     293.69
 H       2.839220     4.217690     1.073682      25.56
 C      -0.023095     3.874299    -0.412118      55.49
 H      -0.192338     3.567299    -1.435892      22.89
 C      -0.454519     5.258122     0.050392     104.04
 O       0.008923     6.387665    -0.751487     220.92
 H      -0.107064     6.134744    -1.750973      26.39
 H      -0.189700     5.157808     1.132190      23.43
 H      -1.563619     5.421963    -0.193092      22.87
 C      -0.951765    -0.674183    -0.117662      59.42
 H      -0.531400    -1.766709    -0.078472      17.85
 C      -2.796164     0.455684    -1.215264      42.23
 H      -3.599771     0.576891    -1.961858      25.47
 C      -2.283366     1.769399    -0.621760       1.17
 O      -3.009411     3.045162    -0.511045      95.57
 C      -4.294939     3.417876    -1.301431     102.91
 H      -5.402317     2.846796    -1.200419      23.77
 H      -4.579748     4.590744    -1.465354      24.67
 H      -3.983097     3.115747    -2.329124      25.30
 C      -1.108617     1.810832     0.054161      22.44
 O      -0.663190     2.926732     0.661426     153.63
 C      -0.515450     0.462504     0.244320      58.59
 H       0.338113     0.680113     0.997460      21.63
 C      -2.264326    -0.786220    -0.805187       8.02
 C      -3.014723    -2.008725    -1.162638      82.43
 H      -3.644140    -1.984951    -2.125879      20.07
 O      -1.826365    -2.931444    -1.688293     224.58
 H      -2.352339    -3.665432    -1.945442      19.43
 C      -3.596724    -2.677861     0.005116      86.83
 H      -2.680041    -2.703354     0.820887      17.27
 O      -4.658792    -1.828269     0.601407     370.24
 H      -4.349700    -1.521722     1.428273      30.13
 C      -4.352607    -3.933364    -0.367109     111.60
 O      -3.850229    -4.899696    -1.248385     394.12
 H      -3.215475    -5.360119    -0.602106      28.36
 H      -5.441197    -3.913854    -0.656780      24.99
 H      -4.559931    -4.367031     0.625008      26.09
55
name = lig-etoh-frame_698
 C       2.019735     2.301028    -2.240341      49.86
 H       1.473110     3.029216    -2.992706      22.61
 C       3.005745     1.622091    -0.090430      59.38
 H       3.601004     1.806121     0.835480      23.79
 C       3.570305     0.475161    -0.861007      18.73
 O       4.556677    -0.348635    -0.302971     225.64
 C       5.498920     0.214320     0.490413     122.22
 H       5.090284     0.733806     1.305328      27.30
 H       6.250934     0.817906    -0.053903      26.73
 H       6.107219    -0.722647     0.806240      25.20
 C       3.211075     0.182226    -2.157007       5.26
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 O       3.940878    -1.011431    -2.856273      93.26
 H       5.054076    -1.036939    -2.459659      22.47
 C       2.626489     1.151117    -2.931257      40.46
 H       2.640089     1.104922    -3.992165      20.54
 C       2.249607     2.522123    -0.836836      31.23
 C       1.563995     3.891996    -0.353002      97.97
 H       1.905238     4.574339    -0.872247      26.59
 O       1.890701     4.017663     1.149549     321.18
 H       2.849117     4.187206     1.195341      26.32
 C       0.028431     3.884101    -0.435872      53.74
 H      -0.280529     3.618021    -1.482677      21.20
 C      -0.520598     5.275764     0.071284      98.85
 O       0.012423     6.365330    -0.814655     212.39
 H      -0.259285     6.272137    -1.824374      25.46
 H      -0.168345     5.522598     1.089965      23.91
 H      -1.568209     5.423032     0.033197      25.30
 C      -1.028424    -0.772547    -0.083760      57.98
 H      -0.497073    -1.620418     0.168243      20.55
 C      -2.776902     0.451931    -1.193424      50.38
 H      -3.543777     0.627849    -2.026708      24.20
 C      -2.325992     1.779654    -0.612955     -21.02
 O      -3.054428     3.058608    -0.447839     101.02
 C      -4.225459     3.354116    -1.358131     117.61
 H      -5.319817     3.217320    -1.151988      25.04
 H      -4.370508     4.460904    -1.024871      25.17
 H      -3.975900     3.323607    -2.419600      26.53
 C      -1.058461     1.757915     0.061630       1.87
 O      -0.675878     2.968922     0.643819     150.87
 C      -0.536716     0.506651     0.249932      67.24
 H       0.487162     0.453010     0.614341      23.50
 C      -2.220858    -0.765371    -0.831589      29.19
 C      -2.885128    -1.984773    -1.232658      89.24
 H      -3.604465    -1.786905    -2.000641      22.77
 O      -1.799521    -2.920273    -1.655213     195.93
 H      -2.216861    -3.896601    -2.078618      15.79
 C      -3.633010    -2.665740     0.003002      93.59
 H      -2.750435    -2.911203     0.513238      22.73
 O      -4.672771    -1.847639     0.542560     317.08
 H      -4.263871    -1.391523     1.523534      22.95
 C      -4.324400    -3.962394    -0.354306     105.00
 O      -3.861362    -4.898474    -1.259005     362.70
 H      -3.274869    -5.646006    -0.824748      27.88
 H      -5.392887    -3.681615    -0.433008      26.68
 H      -4.519026    -4.423189     0.735089      25.86
55
name = lig-etoh-frame_699
 C       2.033899     2.306999    -2.230887      46.75
 H       1.623692     2.991723    -2.877070      24.57
 C       3.052074     1.561499    -0.076295      65.17
 H       3.670269     1.776249     0.778127      23.16
 C       3.606254     0.538346    -0.883141      19.46
 O       4.537359    -0.382530    -0.278401     268.25
 C       5.476230     0.200768     0.466657     121.37
 H       5.003290     0.893143     1.274601      24.40
 H       6.333679     0.984806     0.199052      25.15
 H       6.184277    -0.547742     0.895791      25.87
 C       3.198065     0.184069    -2.134482       9.01
 O       3.894781    -1.011241    -2.871613     184.06
 H       4.706514    -1.106194    -2.392227      25.98
 C       2.626670     1.164356    -2.924202      38.30
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 H       2.626424     1.179990    -4.037167      20.72
 C       2.240983     2.513218    -0.871579      23.98
 C       1.583837     3.849909    -0.267526      78.90
 H       1.951797     4.949538    -1.051862      18.76
 O       1.927199     4.005794     1.103784     296.24
 H       2.891705     4.245915     1.382305      24.44
 C       0.049136     3.914803    -0.408749      69.63
 H      -0.447341     3.690871    -1.356887      21.81
 C      -0.569987     5.320486     0.045175      93.24
 O       0.014512     6.345865    -0.867667     200.42
 H      -0.236632     6.296429    -1.746537      30.10
 H      -0.128444     5.812875     0.925547      23.66
 H      -1.731893     5.168596     0.308901      23.37
 C      -1.119794    -0.847597    -0.052914      14.56
 H      -0.422578    -1.632795     0.417732      18.52
 C      -2.780126     0.560916    -1.169193      68.06
 H      -3.570431     0.464106    -1.867582      24.15
 C      -2.390698     1.758105    -0.602186       5.18
 O      -3.111539     3.024033    -0.419610     154.34
 C      -4.127539     3.340055    -1.388617     110.60
 H      -5.181660     3.006563    -0.937172      23.68
 H      -4.054086     4.499734    -0.877188      21.86
 H      -3.950362     3.438270    -2.478389      24.89
 C      -1.094426     1.727468     0.055345      -3.18
 O      -0.645189     3.011986     0.595837     147.70
 C      -0.459454     0.530284     0.291441      29.08
 H       0.618179     0.340069     0.420835      22.64
 C      -2.169514    -0.715212    -0.866865      27.46
 C      -2.774299    -2.017673    -1.318622      85.28
 H      -3.606200    -1.646948    -2.038346      22.48
 O      -1.780318    -2.925233    -1.636487     279.29
 H      -2.125393    -3.693499    -1.995701      23.41
 C      -3.642259    -2.639541    -0.043524      79.63
 H      -2.767281    -3.105802     0.681517      18.92
 O      -4.663168    -1.846554     0.506734     352.99
 H      -4.455120    -1.630696     1.374137      31.12
 C      -4.370958    -3.998343    -0.259542      88.09
 O      -3.862116    -4.916558    -1.309100     357.80
 H      -3.409670    -5.619629    -0.881596      31.64
 H      -5.330317    -3.504915    -0.599653      26.52
 H      -4.295885    -4.561259     0.690600      27.85
55
name = lig-etoh-frame_700
 C       2.081096     2.268738    -2.246747      39.11
 H       1.590576     3.177627    -2.786068      22.25
 C       3.094888     1.545975    -0.131747      62.14
 H       3.440900     1.895317     0.868453      22.19
 C       3.648734     0.559215    -0.828753      26.71
 O       4.486132    -0.430124    -0.308169     248.70
 C       5.543643     0.254676     0.548625     110.44
 H       5.049518     0.736459     1.346543      27.07
 H       6.086099     1.007598    -0.058038      26.89
 H       6.112698    -0.517533     1.093541      26.35
 C       3.251634     0.127031    -2.209671       3.75
 O       3.798441    -0.963997    -2.861795     170.63
 H       4.603861    -1.270468    -2.201998      21.53
 C       2.586123     1.211175    -2.909010      62.98
 H       2.552648     1.109244    -4.046247      20.71
 C       2.224788     2.528554    -0.866717      25.90
 C       1.648104     3.824836    -0.231928     105.88
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 H       1.863385     4.583141    -0.723773      24.46
 O       1.959193     4.001738     1.078735     329.72
 H       2.887577     4.313929     1.202282      27.04
 C       0.016384     3.961845    -0.320100      65.23
 H      -0.357769     3.758765    -1.354167      21.21
 C      -0.584315     5.373916     0.012160     107.53
 O      -0.007014     6.335036    -0.899426     234.52
 H      -0.182862     6.182193    -1.967474      23.23
 H      -0.117315     5.748612     0.951249      23.82
 H      -1.570770     5.104153     0.188649      25.40
 C      -1.098177    -0.789525     0.035519      27.09
 H      -0.707545    -1.784166     0.372961      17.62
 C      -2.810666     0.645127    -1.167105      59.67
 H      -3.825408     0.377543    -1.670998      22.71
 C      -2.437089     1.763381    -0.549151      26.93
 O      -3.128641     2.923558    -0.419369     229.99
 C      -4.054387     3.396917    -1.345940     123.23
 H      -4.911210     2.740568    -1.091291      24.55
 H      -4.085174     4.529751    -1.244143      24.64
 H      -3.843909     3.306599    -2.434971      25.37
 C      -1.143823     1.746340     0.069076     -21.42
 O      -0.599289     3.021988     0.532131     170.13
 C      -0.387785     0.463611     0.315807      16.07
 H       0.753488     0.514295     0.501280      20.47
 C      -2.147550    -0.681620    -0.913297       4.72
 C      -2.764358    -2.029398    -1.365032      79.38
 H      -3.401590    -1.872248    -2.240333      21.39
 O      -1.731810    -2.924475    -1.633826     230.69
 H      -2.291020    -3.780091    -1.981162      15.64
 C      -3.580433    -2.665316    -0.081674     103.91
 H      -2.964624    -2.763667     0.764539      23.17
 O      -4.653647    -1.832075     0.458562     320.88
 H      -4.557243    -1.804856     1.568551      24.42
 C      -4.425188    -4.021102    -0.210689      92.43
 O      -3.880905    -4.915490    -1.378254     326.61
 H      -3.365718    -5.568583    -0.732056      24.84
 H      -5.388220    -3.794819    -0.721386      25.43
 H      -4.375771    -4.630161     0.728946      28.05
55
name = lig-etoh-frame_701
 C       2.093972     2.312173    -2.237914      43.94
 H       1.570592     3.110961    -2.736356      19.16
 C       3.086998     1.649066    -0.182672      66.84
 H       3.108795     1.864736     0.900596      17.95
 C       3.681020     0.469417    -0.847258      35.34
 O       4.472037    -0.470023    -0.310945     197.39
 C       5.592607     0.295600     0.630562      72.93
 H       4.999158     0.740590     1.504117      24.87
 H       5.953039     0.901176    -0.243840      24.47
 H       6.177802    -0.613677     1.098453      24.66
 C       3.309975     0.162460    -2.265444      16.70
 O       3.715666    -0.911121    -2.836832     104.70
 H       4.267564    -1.594870    -2.143713      20.95
 C       2.571675     1.169439    -2.928824      66.03
 H       2.402976     1.072093    -3.958046      23.80
 C       2.237926     2.509581    -0.843986      46.45
 C       1.650873     3.749717    -0.225454      90.22
 H       2.134947     4.844560    -0.956567      19.48
 O       2.006625     4.004228     1.111332     287.29
 H       2.933968     4.348003     1.014397      27.44
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 C      -0.004849     3.994212    -0.267763      71.91
 H      -0.086065     3.834622    -1.365938      20.08
 C      -0.519831     5.403534    -0.004260     101.33
 O      -0.055386     6.339706    -0.947991     301.84
 H       0.046044     5.995039    -1.869965      26.86
 H      -0.259257     5.590501     1.039108      23.75
 H      -1.740573     5.325375    -0.129353      22.52
 C      -1.051432    -0.684363     0.093131      46.20
 H      -0.923017    -1.778344     0.238020      17.46
 C      -2.881458     0.581783    -1.197164      43.95
 H      -3.907592     0.614657    -1.440493      23.56
 C      -2.428389     1.784163    -0.468233      17.92
 O      -3.116986     2.849998    -0.401196     206.50
 C      -4.011011     3.436288    -1.334441     110.72
 H      -4.981244     2.713953    -1.473257      23.42
 H      -4.308411     4.654344    -1.375235      22.76
 H      -3.570356     3.044821    -2.311050      23.77
 C      -1.125839     1.749005     0.104961      -2.25
 O      -0.571148     2.982856     0.495584     192.77
 C      -0.358908     0.446775     0.328602      40.14
 H       0.587204     0.655131     0.736933      19.98
 C      -2.150907    -0.631883    -0.933506      -0.56
 C      -2.803225    -2.012734    -1.361578      71.74
 H      -3.302221    -2.102710    -2.390672      18.21
 O      -1.670585    -2.959309    -1.654919     208.82
 H      -2.314582    -3.811754    -1.811980      14.45
 C      -3.561859    -2.704108    -0.101617      77.72
 H      -2.787012    -2.455700     0.795829      16.40
 O      -4.645403    -1.787807     0.424176     285.22
 H      -4.666334    -2.036725     1.462434      25.85
 C      -4.445389    -4.036857    -0.255241      92.56
 O      -3.897562    -4.918522    -1.410663     343.29
 H      -3.192463    -5.425667    -0.884092      27.44
 H      -5.507163    -4.004043    -0.512910      26.66
 H      -4.657663    -4.597018     0.773235      26.46
55
name = lig-etoh-frame_702
 C       2.091364     2.355069    -2.234147      49.47
 H       1.495286     3.046477    -2.872180      20.89
 C       3.095943     1.699768    -0.206303      72.55
 H       3.016708     1.693014     0.878007      20.64
 C       3.651472     0.416828    -0.907456      13.13
 O       4.497614    -0.510247    -0.259603     200.14
 C       5.588051     0.272480     0.691748      82.86
 H       5.085021     0.891363     1.411169      26.54
 H       6.106865     0.903214    -0.134188      25.73
 H       6.285598    -0.468183     0.885720      27.21
 C       3.355916     0.298502    -2.221561      31.59
 O       3.659479    -0.939713    -2.839029     255.83
 H       3.947246    -1.510605    -2.271466      28.69
 C       2.555114     1.136600    -2.943173      45.44
 H       2.183310     1.007938    -4.054302      21.94
 C       2.244451     2.500628    -0.864783      51.88
 C       1.630054     3.774672    -0.255047     106.07
 H       2.052498     4.434234    -0.831111      26.59
 O       2.067626     4.008276     1.158121     265.89
 H       3.070644     4.324837     1.131171      26.86
 C       0.050875     3.985666    -0.308221      68.92
 H      -0.086100     3.826976    -1.392151      21.93
 C      -0.507917     5.396439    -0.021347     113.34
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 O      -0.084951     6.366903    -0.967062     310.63
 H       0.165528     5.926867    -1.849497      26.47
 H      -0.431774     5.710427     1.058993      24.37
 H      -1.491695     5.527350    -0.258937      25.44
 C      -1.064034    -0.625075     0.048220      35.17
 H      -0.738663    -1.745723     0.247722      18.30
 C      -2.924877     0.519819    -1.170856      44.35
 H      -4.009376     0.721478    -1.453878      22.81
 C      -2.366584     1.688399    -0.438071      -2.35
 O      -3.141911     2.884171    -0.333846     161.90
 C      -3.983229     3.391463    -1.411194     117.35
 H      -5.016924     3.020886    -1.547220      25.73
 H      -4.377256     4.471670    -1.229729      24.91
 H      -3.320517     3.200109    -2.230906      24.93
 C      -1.070664     1.730472     0.123848      28.95
 O      -0.559108     2.922345     0.509605     173.27
 C      -0.370579     0.543947     0.353882      35.93
 H       0.521724     0.619580     1.151609      20.29
 C      -2.194634    -0.593731    -0.924263      17.29
 C      -2.821798    -2.011998    -1.342224      74.44
 H      -3.411258    -2.015445    -2.269525      20.54
 O      -1.628592    -3.007173    -1.660423     238.42
 H      -2.048312    -3.797782    -1.761948      23.09
 C      -3.591576    -2.687239    -0.090196      95.76
 H      -2.728820    -2.751849     0.499018      24.11
 O      -4.636950    -1.747977     0.388397     338.95
 H      -4.734901    -1.973458     1.261415      28.74
 C      -4.439945    -4.069020    -0.331152      92.91
 O      -3.910641    -4.911315    -1.407010     393.65
 H      -3.131308    -5.395384    -1.072112      30.50
 H      -5.535076    -3.764735    -0.449392      27.08
 H      -4.551022    -4.563550     0.660643      27.75
55
name = lig-etoh-frame_703
 C       2.081962     2.341341    -2.308321      41.52
 H       1.381746     2.994079    -2.937169      20.79
 C       3.141923     1.621439    -0.213249      64.85
 H       3.141177     1.567912     0.906644      20.89
 C       3.619700     0.468243    -0.864562      15.57
 O       4.534448    -0.522633    -0.179663     243.50
 C       5.553385     0.239575     0.663360      96.08
 H       5.176855     0.943731     1.445464      25.91
 H       6.192741     0.976969     0.118572      26.58
 H       6.468192    -0.516615     0.940725      24.72
 C       3.400655     0.347341    -2.218089      11.12
 O       3.601970    -0.952274    -2.877348     136.71
 H       3.929973    -1.666107    -2.022537      19.96
 C       2.493583     1.204318    -2.951130      52.56
 H       2.184823     0.883804    -3.872656      23.44
 C       2.224181     2.535928    -0.905468      48.39
 C       1.600389     3.794829    -0.211686      85.64
 H       2.170033     4.689471    -1.079751      20.24
 O       2.118266     4.011104     1.183508     261.80
 H       3.072678     4.216616     1.317596      26.52
 C       0.132119     3.936971    -0.384791      60.08
 H      -0.306257     3.724686    -1.394819      21.92
 C      -0.519773     5.377065    -0.029816      92.42
 O      -0.069843     6.420671    -0.957601     211.96
 H       0.135177     6.071767    -1.964088      24.17
 H      -0.394446     5.873381     0.908033      23.48
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 H      -1.728613     5.273802    -0.202143      22.83
 C      -1.085515    -0.607211    -0.062694      25.39
 H      -0.514855    -1.437381     0.253721      20.61
 C      -2.960985     0.554712    -1.082548      61.93
 H      -3.902353     0.535504    -1.630805      23.29
 C      -2.349183     1.596292    -0.465844       0.01
 O      -3.175356     2.932788    -0.246731      97.09
 C      -3.930820     3.307621    -1.488763      99.28
 H      -5.063857     2.994472    -1.565262      23.82
 H      -4.147970     4.545994    -1.070818      22.69
 H      -3.304350     3.540426    -2.422598      24.33
 C      -1.036309     1.733601     0.104505      13.68
 O      -0.537216     2.900919     0.560592     140.23
 C      -0.385307     0.616828     0.431961      32.08
 H       0.291383     0.471707     1.142798      22.94
 C      -2.235141    -0.658985    -0.888833      14.29
 C      -2.810632    -2.038441    -1.308756      72.14
 H      -3.554211    -1.805671    -2.143331      21.61
 O      -1.604863    -3.006499    -1.642794     145.96
 H      -1.964776    -4.063643    -1.841392      15.97
 C      -3.651414    -2.656293    -0.113316      81.87
 H      -2.761182    -3.211302     0.540357      17.50
 O      -4.605003    -1.712382     0.334504     262.40
 H      -4.858941    -1.821248     1.465529      22.40
 C      -4.421509    -4.064282    -0.404986      79.22
 O      -3.941229    -4.889793    -1.407976     357.32
 H      -3.157362    -5.489719    -0.992645      26.08
 H      -5.330446    -3.573021    -0.696544      28.22
 H      -4.222979    -4.668071     0.599137      26.42
55
name = lig-etoh-frame_704
 C       2.020378     2.360062    -2.373353      33.02
 H       1.346079     2.978665    -2.860596      21.67
 C       3.127895     1.559795    -0.202366      59.07
 H       3.333950     1.641400     0.842764      21.12
 C       3.651941     0.513716    -0.786793      15.98
 O       4.561051    -0.484269    -0.097764     252.24
 C       5.555379     0.194936     0.613689     120.32
 H       5.159160     0.645571     1.580743      27.05
 H       6.142490     1.059106     0.099438      27.01
 H       6.150574    -0.481183     1.087649      28.89
 C       3.400817     0.309890    -2.280745       7.25
 O       3.556685    -0.951055    -2.878605     166.77
 H       3.986472    -1.509367    -2.155413      22.26
 C       2.489116     1.234452    -2.931236      59.46
 H       2.162946     0.778792    -3.945616      22.57
 C       2.243123     2.554737    -0.925860      36.38
 C       1.678401     3.843766    -0.205490      99.94
 H       1.887496     4.679199    -0.770130      25.30
 O       2.104590     4.003755     1.183726     265.58
 H       3.161071     4.155514     1.215807      24.62
 C       0.146287     3.898042    -0.416161      55.78
 H      -0.281004     3.594851    -1.371515      23.42
 C      -0.572580     5.349455    -0.083114     100.76
 O      -0.039448     6.473650    -0.945128     206.79
 H      -0.087089     6.284763    -1.886213      28.39
 H      -0.233156     5.823280     0.898889      22.71
 H      -1.523658     4.940476    -0.024647      24.30
 C      -1.066010    -0.571513    -0.162470      38.25
 H      -0.311748    -1.453843     0.181941      21.77
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 C      -2.983402     0.544104    -1.000115      55.12
 H      -3.815920     0.461693    -1.690709      23.07
 C      -2.375328     1.646258    -0.484303       5.06
 O      -3.190456     2.928933    -0.209784     142.00
 C      -3.889366     3.311298    -1.509035     117.45
 H      -4.786721     2.764648    -1.645515      26.84
 H      -3.894652     4.317022    -1.137908      25.15
 H      -3.466110     3.478145    -2.500186      26.90
 C      -1.039903     1.774275     0.074512      -5.41
 O      -0.502261     2.934790     0.623605     130.27
 C      -0.463333     0.567152     0.472980      28.47
 H       0.463854     0.365952     1.209427      22.75
 C      -2.250795    -0.760894    -0.837012      19.98
 C      -2.793474    -2.082343    -1.269267      89.63
 H      -3.494281    -1.795700    -2.091097      22.22
 O      -1.616435    -2.989486    -1.617267     251.22
 H      -2.012983    -3.829173    -1.904719      21.12
 C      -3.651001    -2.692965    -0.134582     108.66
 H      -3.106104    -3.008142     0.678510      23.09
 O      -4.574888    -1.677366     0.316496     356.70
 H      -4.714889    -1.669260     1.236184      30.73
 C      -4.390247    -4.006556    -0.446785     104.15
 O      -3.948331    -4.893633    -1.440484     384.71
 H      -3.442200    -5.464636    -0.889121      31.31
 H      -5.432044    -3.717013    -0.890311      26.29
 H      -4.387891    -4.547182     0.462485      29.51
55
name = lig-etoh-frame_705
 C       1.950143     2.409449    -2.330034      59.85
 H       1.199707     3.140366    -2.914719      20.28
 C       3.045414     1.605795    -0.173311      54.80
 H       3.450099     1.907116     0.848324      22.44
 C       3.735759     0.463358    -0.817117      19.94
 O       4.542952    -0.422074    -0.060533     261.15
 C       5.570271     0.187347     0.623337     109.62
 H       5.056129     0.490488     1.567945      24.29
 H       6.032924     0.911850    -0.000701      26.83
 H       6.156323    -0.758072     1.139716      23.83
 C       3.359484     0.265974    -2.284759      15.29
 O       3.528502    -0.931508    -2.871876     170.07
 H       4.131961    -1.451907    -2.287147      23.91
 C       2.537659     1.163176    -2.952034      46.86
 H       2.171466     0.932013    -3.934569      23.53
 C       2.300343     2.560808    -0.947870      28.95
 C       1.762183     3.842118    -0.213866      88.57
 H       1.861904     5.076751    -0.680948      20.16
 O       2.071850     3.989376     1.165146     310.84
 H       3.008367     4.177960     1.100909      26.82
 C       0.120552     3.877888    -0.375484      62.08
 H      -0.037958     3.480135    -1.414185      20.75
 C      -0.544800     5.312264    -0.133840      96.56
 O      -0.031718     6.506780    -0.912936     171.91
 H      -0.350183     6.377111    -1.949410      23.22
 H      -0.196912     5.469782     0.870432      24.49
 H      -1.689460     4.952585    -0.016379      22.75
 C      -0.968496    -0.602551    -0.197915      54.19
 H      -0.513145    -1.508685    -0.148448      22.72
 C      -2.975748     0.442250    -0.941007      30.63
 H      -3.922034     0.573836    -1.581485      21.00
 C      -2.410279     1.798674    -0.461995      -0.81
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 O      -3.175270     2.872005    -0.242779     190.23
 C      -3.846143     3.339981    -1.490779      88.14
 H      -4.716322     2.496507    -1.662284      22.18
 H      -4.147439     4.573811    -1.249688      22.41
 H      -3.257165     3.133889    -2.483193      24.28
 C      -1.059527     1.804241     0.089942     -12.25
 O      -0.467380     2.992820     0.667712     157.71
 C      -0.551093     0.493973     0.479982      55.04
 H       0.404699     0.469962     0.893040      24.08
 C      -2.260440    -0.778109    -0.784508      19.76
 C      -2.762473    -2.134248    -1.232601      89.08
 H      -3.373413    -2.035557    -2.181140      20.97
 O      -1.653833    -2.943589    -1.590785     270.03
 H      -2.165407    -3.722462    -1.967487      19.85
 C      -3.639582    -2.730611    -0.132497      94.29
 H      -3.049551    -2.678530     0.941543      18.07
 O      -4.553483    -1.637144     0.271706     322.52
 H      -4.536758    -1.651762     1.331375      26.10
 C      -4.437653    -3.919303    -0.505278     106.87
 O      -3.930693    -4.912949    -1.491701     322.32
 H      -3.471202    -5.629747    -0.887555      27.00
 H      -5.449650    -3.832624    -0.779606      27.86
 H      -4.860715    -4.435086     0.523775      25.92
55
name = lig-etoh-frame_706
 C       1.924190     2.390525    -2.277219      71.11
 H       1.377075     3.046734    -2.800939      25.20
 C       3.018048     1.647493    -0.177834      70.45
 H       3.343599     2.102746     0.728466      23.52
 C       3.760596     0.462522    -0.874851      15.43
 O       4.474134    -0.387048    -0.090674     239.89
 C       5.597954     0.142973     0.718587     103.42
 H       5.148858     0.761084     1.566468      23.77
 H       6.186733     0.857438    -0.017202      25.27
 H       6.246525    -0.643964     0.799321      26.53
 C       3.313316     0.232943    -2.197286      16.88
 O       3.520262    -0.935007    -2.870105     146.66
 H       4.491907    -1.474856    -2.497055      21.37
 C       2.539775     1.169164    -2.958021      29.97
 H       2.239965     0.987497    -4.007755      22.26
 C       2.345981     2.605855    -0.962989      15.51
 C       1.768971     3.884608    -0.248161     102.22
 H       2.067829     4.776684    -0.705623      24.63
 O       2.035854     3.965944     1.140819     308.05
 H       3.025680     4.296894     1.286715      25.07
 C       0.125785     3.861842    -0.339624      76.71
 H       0.066531     3.412315    -1.323478      21.63
 C      -0.504342     5.246430    -0.164959     104.38
 O      -0.064791     6.503235    -0.872959     262.68
 H      -0.272924     6.353532    -1.786638      29.62
 H      -0.243051     5.331387     0.934757      23.75
 H      -1.553999     5.412596    -0.259102      24.49
 C      -0.917661    -0.704083    -0.223558      37.96
 H      -0.409024    -1.787503    -0.365385      18.13
 C      -2.959326     0.407172    -0.888731      31.42
 H      -3.937761     0.500656    -1.235705      21.78
 C      -2.395763     1.838801    -0.424663       9.47
 O      -3.178274     2.859962    -0.306628     229.59
 C      -3.823843     3.353934    -1.472983     130.09
 H      -4.638796     2.750562    -1.591162      27.49
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 H      -4.455898     4.217371    -1.644282      25.85
 H      -3.010116     3.069542    -2.087967      25.66
 C      -1.117047     1.814247     0.152955      -4.25
 O      -0.444567     3.034673     0.684194     176.30
 C      -0.601053     0.499218     0.439735      45.29
 H       0.512369     0.584174     0.746854      22.01
 C      -2.259835    -0.726638    -0.753900      21.03
 C      -2.748449    -2.147942    -1.215055      91.10
 H      -3.350886    -2.194374    -2.159895      19.88
 O      -1.676876    -2.920664    -1.568402     215.75
 H      -2.190194    -3.789543    -2.072822      16.09
 C      -3.614664    -2.708173    -0.069877     106.16
 H      -2.895935    -2.828867     0.680528      23.75
 O      -4.555973    -1.601497     0.234130     337.25
 H      -4.372800    -1.610039     1.334455      23.82
 C      -4.545692    -3.907193    -0.520838      87.78
 O      -3.908117    -4.928742    -1.521305     310.60
 H      -3.362258    -5.622379    -1.012368      28.22
 H      -5.553847    -3.462306    -0.977943      27.08
 H      -4.893775    -4.341521     0.351677      27.56
55
name = lig-etoh-frame_707
 C       1.977457     2.277549    -2.260026      80.37
 H       1.407558     3.126325    -2.883508      24.75
 C       3.062376     1.670842    -0.244873      61.12
 H       3.279085     2.052520     0.799424      22.33
 C       3.702193     0.565187    -0.871917      28.39
 O       4.414238    -0.384580    -0.130880     219.40
 C       5.610802     0.149793     0.760916     106.86
 H       5.439358     0.816570     1.592657      26.18
 H       6.228198     0.796589     0.203909      27.97
 H       6.394307    -0.732890     0.812290      24.72
 C       3.261008     0.211528    -2.123746      22.28
 O       3.571816    -0.968940    -2.866147     239.59
 H       4.367814    -1.259293    -2.737859      32.03
 C       2.494123     1.240790    -2.914895      40.90
 H       2.404410     0.940725    -4.002645      20.67
 C       2.354415     2.663089    -0.945667      18.84
 C       1.718066     3.893618    -0.264287      86.77
 H       2.302415     4.723236    -1.029060      19.88
 O       2.023993     3.950388     1.132931     323.50
 H       2.871662     4.350907     1.433635      26.77
 C       0.174265     3.848139    -0.355292      74.78
 H      -0.139291     3.362568    -1.305096      21.57
 C      -0.468241     5.223316    -0.158006     101.71
 O      -0.084193     6.478374    -0.804941     228.00
 H      -0.065589     6.233822    -1.864840      25.21
 H      -0.406517     5.496926     0.902676      23.91
 H      -1.541467     5.454366    -0.478805      20.99
 C      -0.915837    -0.812064    -0.240661      33.92
 H      -0.215191    -1.562511    -0.276821      20.22
 C      -2.940500     0.505996    -0.819371      37.71
 H      -4.098599     0.316816    -0.940502      18.98
 C      -2.368031     1.729935    -0.397355      15.64
 O      -3.215280     2.927119    -0.316252     195.37
 C      -3.808043     3.304144    -1.500318     100.24
 H      -4.800077     2.605453    -1.757511      23.20
 H      -4.408284     4.418612    -1.665015      23.06
 H      -2.937858     3.324611    -2.283628      23.63
 C      -1.173752     1.814380     0.246254       2.84
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 O      -0.444211     3.033580     0.690003     180.02
 C      -0.544775     0.522964     0.368201       8.31
 H       0.493433     0.648376     0.727977      21.33
 C      -2.218248    -0.729754    -0.757989      12.18
 C      -2.790821    -2.104782    -1.212556      90.70
 H      -3.513376    -1.995410    -2.055879      20.86
 O      -1.663125    -2.957133    -1.568462     291.88
 H      -1.973599    -3.679865    -1.933085      25.54
 C      -3.615828    -2.673860    -0.057488      82.53
 H      -2.775400    -3.195971     0.707932      19.18
 O      -4.546707    -1.587398     0.244891     372.99
 H      -4.526460    -1.427169     1.115365      33.02
 C      -4.644868    -3.895649    -0.563132      72.69
 O      -3.905803    -4.915307    -1.533196     302.27
 H      -3.291484    -5.407512    -0.960924      27.40
 H      -5.202469    -3.259375    -1.194859      28.57
 H      -4.945309    -4.563394     0.411261      24.95
55
name = lig-etoh-frame_708
 C       2.006291     2.278228    -2.258256      77.19
 H       1.504305     2.952167    -2.864066      28.65
 C       3.134522     1.755803    -0.280035      67.57
 H       3.287693     1.709088     0.799183      21.89
 C       3.628000     0.648775    -0.828302      42.30
 O       4.395019    -0.374731    -0.138075     174.91
 C       5.630036     0.140780     0.738992      99.42
 H       5.437836     0.603249     1.796973      26.31
 H       6.260586     0.909213     0.107825      26.35
 H       6.111743    -0.750035     1.118163      26.64
 C       3.201426     0.212755    -2.137527      23.32
 O       3.604375    -0.968734    -2.851502     130.91
 H       4.701400    -1.214398    -2.708760      25.73
 C       2.497466     1.191830    -2.870222      46.97
 H       2.423376     1.017058    -3.891616      20.31
 C       2.335300     2.663528    -0.919681      24.35
 C       1.705494     3.879041    -0.302120     106.80
 H       1.866747     4.698624    -0.885811      22.18
 O       2.000520     3.946194     1.135094     304.86
 H       2.883758     4.381401     1.253646      25.65
 C       0.201448     3.843432    -0.408290      49.32
 H      -0.283257     3.468332    -1.322514      21.74
 C      -0.500401     5.258786    -0.133523      99.31
 O      -0.063064     6.448893    -0.770607     259.84
 H       0.210035     6.212413    -1.710993      28.66
 H      -0.563777     5.568233     0.915944      23.00
 H      -1.509513     4.811862    -0.453526      22.40
 C      -0.917765    -0.779309    -0.212473      35.96
 H      -0.020250    -1.512246    -0.138641      17.30
 C      -2.948399     0.563153    -0.749398      55.41
 H      -3.950155     0.391956    -0.764263      21.02
 C      -2.421436     1.672926    -0.362498       1.72
 O      -3.237831     2.987521    -0.293304     165.51
 C      -3.843944     3.268381    -1.618383     121.10
 H      -4.501206     2.590811    -1.956215      27.27
 H      -3.922662     4.284108    -1.219258      23.56
 H      -3.291806     3.529083    -2.517004      26.86
 C      -1.151976     1.781344     0.348909       6.01
 O      -0.466814     2.991460     0.696981     160.97
 C      -0.436197     0.530112     0.277660       6.59
 H       0.548107     0.597752     0.760394      18.66
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 C      -2.170059    -0.766438    -0.787242      12.22
 C      -2.840792    -2.047545    -1.219390      76.89
 H      -3.591303    -1.728350    -2.011021      20.24
 O      -1.635025    -2.971467    -1.564845     174.75
 H      -2.039492    -3.929818    -1.935020      16.95
 C      -3.629901    -2.694152    -0.055333      96.25
 H      -3.120548    -3.179078     0.710067      23.25
 O      -4.529307    -1.594900     0.262686     317.50
 H      -4.739032    -1.234248     1.314290      26.08
 C      -4.647862    -3.897715    -0.603146      90.44
 O      -3.926079    -4.870542    -1.521497     322.38
 H      -3.223211    -5.204521    -0.791898      25.06
 H      -5.241924    -3.317138    -1.403324      27.15
 H      -5.170321    -4.433338     0.088295      29.03
55
name = lig-etoh-frame_709
 C       2.020944     2.358673    -2.234673      29.04
 H       1.402290     3.000754    -2.945978      19.56
 C       3.215092     1.861414    -0.223814      99.02
 H       3.339131     1.685198     0.839697      17.95
 C       3.587275     0.604965    -0.830894      52.43
 O       4.405964    -0.333356    -0.116361     236.47
 C       5.610497     0.134187     0.711800     101.47
 H       5.133633     0.461657     1.609904      28.45
 H       6.191197     0.759963     0.122080      29.81
 H       5.962341    -0.877720     1.109522      26.36
 C       3.194964     0.204118    -2.161755      14.48
 O       3.654387    -0.951507    -2.821109     172.37
 H       4.650234    -1.087794    -2.461667      22.13
 C       2.517517     1.074712    -2.852442      55.02
 H       2.292204     1.068254    -3.990591      23.80
 C       2.296648     2.650016    -0.935263      80.53
 C       1.682795     3.825856    -0.309307     115.05
 H       1.678028     5.023254    -0.759491      19.18
 O       1.978518     3.963319     1.121294     216.84
 H       2.963171     4.293641     1.033561      30.46
 C       0.169577     3.848554    -0.425507      39.80
 H      -0.155186     3.577374    -1.443646      20.68
 C      -0.580728     5.250084    -0.100370     109.43
 O      -0.020293     6.418534    -0.752470     233.19
 H       0.243387     6.230226    -1.651365      30.26
 H      -0.668256     5.446024     1.000032      24.58
 H      -1.466705     4.666884    -0.335138      23.31
 C      -0.863830    -0.663426    -0.162887      43.10
 H      -0.257101    -1.572200    -0.108274      18.32
 C      -2.954088     0.463454    -0.709099      24.97
 H      -4.133758     0.526343    -0.837087      18.46
 C      -2.449748     1.773912    -0.248411     -18.65
 O      -3.224084     2.979290    -0.296706     146.00
 C      -3.849936     3.297780    -1.703290      81.66
 H      -4.683920     2.439048    -2.068855      22.24
 H      -4.153689     4.288708    -1.127110      21.84
 H      -3.226929     3.485108    -2.640587      24.26
 C      -1.093244     1.716369     0.386600       6.77
 O      -0.497566     2.934225     0.700665     129.67
 C      -0.327809     0.548414     0.213526      40.02
 H       0.703393     0.457092     0.749197      16.67
 C      -2.148162    -0.759465    -0.800748      19.75
 C      -2.848627    -2.015513    -1.220328      72.60
 H      -3.498155    -1.768733    -2.060026      21.49
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 O      -1.638180    -2.982610    -1.580110     190.51
 H      -2.194149    -3.846684    -1.791772      17.41
 C      -3.723766    -2.728620    -0.074752      82.30
 H      -3.143191    -3.055286     0.954975      20.28
 O      -4.531584    -1.590655     0.304465     346.93
 H      -4.697078    -1.552139     1.304981      28.05
 C      -4.610400    -3.850661    -0.719255     102.21
 O      -3.934941    -4.812730    -1.462122     338.71
 H      -3.294373    -5.265878    -0.907749      30.19
 H      -5.430459    -3.520831    -1.341551      26.68
 H      -5.521980    -4.297930     0.013993      25.06
55
name = lig-etoh-frame_710
 C       2.043877     2.373778    -2.284092       9.83
 H       1.312024     3.033090    -2.854088      18.82
 C       3.294451     1.876712    -0.174087      74.86
 H       3.404205     2.105251     0.951273      13.82
 C       3.581657     0.552761    -0.812343      23.17
 O       4.421245    -0.291978    -0.108730     277.35
 C       5.513771     0.080431     0.694854      94.84
 H       4.936418     0.717043     1.492415      24.50
 H       6.335519     0.731239     0.155268      25.89
 H       6.049843    -0.907622     0.834185      25.29
 C       3.257856     0.149158    -2.144808       5.03
 O       3.717033    -0.931023    -2.768920     217.60
 H       4.495772    -1.157976    -2.278724      23.46
 C       2.447568     1.098404    -2.888411      53.64
 H       2.225666     0.891564    -3.897471      26.28
 C       2.283286     2.662443    -0.942179      72.31
 C       1.607641     3.851117    -0.278377     124.60
 H       1.965973     4.728997    -0.677569      23.51
 O       1.976656     3.992392     1.080804     297.74
 H       2.936183     4.122040     1.206451      30.70
 C       0.102731     3.852148    -0.397736      52.36
 H      -0.017766     3.576855    -1.476812      19.69
 C      -0.644932     5.178438    -0.056207      90.87
 O       0.012367     6.382333    -0.724716     190.66
 H       0.071779     6.137901    -1.797064      26.29
 H      -0.609180     5.344358     1.002488      24.72
 H      -1.819340     5.198277    -0.411551      22.20
 C      -0.834709    -0.586820    -0.158205      45.88
 H      -0.439758    -1.611893    -0.112205      18.28
 C      -2.976781     0.393167    -0.662905      28.15
 H      -3.933696     0.481331    -1.115873      20.70
 C      -2.438350     1.815769    -0.116379     -15.41
 O      -3.191145     2.933487    -0.333610     171.11
 C      -3.877408     3.338518    -1.736849      95.75
 H      -4.611193     2.683466    -1.857944      26.39
 H      -4.725087     4.136735    -1.701927      23.95
 H      -3.006761     3.356526    -2.381189      24.61
 C      -1.068353     1.696474     0.337358      10.13
 O      -0.514606     2.892763     0.697349     153.56
 C      -0.201513     0.567757     0.211955      52.46
 H       0.751863     0.508957     0.566731      17.63
 C      -2.152460    -0.686693    -0.766758      29.32
 C      -2.788598    -2.032705    -1.201949      66.09
 H      -3.386138    -1.978390    -2.189791      19.85
 O      -1.686048    -2.978823    -1.598801     259.92
 H      -2.208123    -3.717486    -1.731268      22.31
 C      -3.827691    -2.733368    -0.090222      83.61
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 H      -3.145454    -2.936261     0.719668      23.74
 O      -4.559444    -1.597654     0.357143     369.26
 H      -4.628532    -1.855486     1.321763      26.25
 C      -4.653389    -3.792198    -0.789276     106.17
 O      -3.925532    -4.774407    -1.412934     373.27
 H      -3.375326    -5.438885    -0.852680      28.31
 H      -5.428759    -3.374065    -1.512002      27.13
 H      -5.227638    -4.132847    -0.009184      27.26
55
name = lig-etoh-frame_711
 C       2.050876     2.334614    -2.351978      30.68
 H       1.344934     2.988107    -2.799344      18.44
 C       3.300006     1.858339    -0.184230      61.30
 H       3.539643     2.361674     0.715028      15.31
 C       3.607872     0.570362    -0.748693      23.15
 O       4.425400    -0.301564    -0.139373     289.46
 C       5.425485     0.070747     0.679372     135.84
 H       5.247941     0.732616     1.514154      28.19
 H       6.207583     0.657323     0.259209      28.36
 H       6.002298    -0.821968     0.937869      27.18
 C       3.279242     0.188485    -2.115932       3.74
 O       3.794794    -0.931170    -2.725523     149.49
 H       4.465707    -1.576265    -1.985795      18.10
 C       2.383960     1.149405    -2.895223      68.78
 H       2.129867     0.710092    -3.916067      25.03
 C       2.325515     2.652600    -0.916399      68.46
 C       1.559147     3.890827    -0.230941     108.56
 H       2.253605     4.634608    -0.954703      21.02
 O       1.965924     4.019358     1.073627     301.55
 H       2.927735     4.082438     1.345733      26.46
 C       0.000406     3.847352    -0.353890      69.28
 H      -0.183549     3.453009    -1.344526      20.18
 C      -0.723004     5.139876    -0.049805     108.85
 O       0.033497     6.317771    -0.711597     208.39
 H      -0.153369     6.107947    -1.599111      31.46
 H      -0.513364     5.318991     1.053640      24.49
 H      -1.614867     5.544737    -0.342680      25.24
 C      -0.832293    -0.585398    -0.197611      36.17
 H      -0.319124    -1.621156    -0.104567      17.26
 C      -2.986870     0.456907    -0.607301      63.26
 H      -3.865576     0.344616    -1.350602      18.01
 C      -2.436879     1.704311    -0.058121      -2.63
 O      -3.171924     2.924154    -0.362165     168.31
 C      -3.901396     3.354216    -1.720750      83.57
 H      -4.596297     2.320475    -1.894641      22.65
 H      -4.649748     4.191840    -2.012241      23.82
 H      -2.946643     3.321534    -2.278290      23.80
 C      -1.060738     1.730398     0.242793       3.14
 O      -0.502400     2.894011     0.685470     190.59
 C      -0.137008     0.582894     0.233844      21.34
 H       1.050679     0.730873     0.459287      13.11
 C      -2.157613    -0.633667    -0.700429      24.74
 C      -2.716335    -2.067870    -1.199811      75.88
 H      -3.281817    -1.950750    -2.110215      20.94
 O      -1.733485    -2.954679    -1.605549     204.80
 H      -2.290958    -3.949860    -1.778258      14.19
 C      -3.858642    -2.654851    -0.173371      66.40
 H      -3.089736    -3.217522     0.619588      18.65
 O      -4.616552    -1.613123     0.426161     310.18
 H      -4.691843    -1.961286     1.526189      20.94
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 C      -4.736264    -3.712348    -0.811097      74.29
 O      -3.888141    -4.775257    -1.401276     279.36
 H      -3.613054    -5.367268    -0.584502      26.35
 H      -5.180417    -3.199993    -1.653968      27.62
 H      -5.204082    -4.232684     0.180865      25.81
55
name = lig-etoh-frame_712
 C       2.031717     2.321556    -2.330301      28.47
 H       1.287387     3.049997    -2.932114      10.97
 C       3.238774     1.853951    -0.243178      41.91
 H       3.837120     2.301269     0.651484      13.36
 C       3.634437     0.634099    -0.729943      29.51
 O       4.412398    -0.365197    -0.179476     253.44
 C       5.421079     0.090598     0.703954     109.91
 H       5.295346     0.631162     1.727964      24.18
 H       6.157226     0.703837     0.034201      26.11
 H       5.859368    -0.849659     1.265890      25.15
 C       3.262404     0.297631    -2.074588      30.57
 O       3.882666    -0.957204    -2.661723     220.69
 H       4.170471    -1.522128    -2.059160      27.31
 C       2.395121     1.095099    -2.894806      66.42
 H       2.002293     0.745701    -3.870342      26.75
 C       2.362361     2.616329    -0.924230      93.73
 C       1.609428     3.919887    -0.262124     104.75
 H       1.847320     4.648273    -0.933439      26.62
 O       1.932892     4.053498     1.118223     286.21
 H       2.951355     4.236963     1.187130      25.91
 C      -0.101886     3.822954    -0.319275      69.17
 H      -0.469444     3.333965    -1.260968      18.14
 C      -0.719787     5.176794    -0.020227      92.89
 O       0.050003     6.239682    -0.681577     207.66
 H      -0.199833     6.134899    -1.713698      26.34
 H      -0.588629     5.312880     1.029950      25.41
 H      -1.890529     5.431804    -0.325204      22.38
 C      -0.787039    -0.619317    -0.226942      40.35
 H      -0.183850    -1.465833    -0.219683      19.41
 C      -3.000119     0.545951    -0.583609      61.63
 H      -3.847963     0.408730    -1.261491      19.92
 C      -2.483452     1.585116    -0.100509       5.13
 O      -3.163735     2.953169    -0.351981     156.64
 C      -3.908591     3.239347    -1.700057     111.84
 H      -4.273801     2.390668    -2.067084      26.74
 H      -4.230279     4.371214    -1.767740      23.80
 H      -3.088986     3.344216    -2.456145      25.11
 C      -1.011410     1.747202     0.165595      -7.62
 O      -0.480347     2.927934     0.675043     210.28
 C      -0.142707     0.608628     0.242629      29.86
 H       0.827100     0.833880     0.322020      16.28
 C      -2.141659    -0.654501    -0.618138      20.15
 C      -2.709730    -2.039483    -1.197784      78.88
 H      -3.335287    -1.602135    -2.103267      20.10
 O      -1.759632    -2.979639    -1.608689     273.13
 H      -2.185719    -3.771562    -1.724734      20.91
 C      -3.788857    -2.573050    -0.226198     102.82
 H      -3.389271    -3.371954     0.363542      19.26
 O      -4.681042    -1.648941     0.524875     392.29
 H      -4.733792    -1.689944     1.399585      33.47
 C      -4.785920    -3.654032    -0.797283      89.00
 O      -3.860191    -4.783738    -1.381462     299.86
 H      -3.662264    -5.199900    -0.581437      29.81
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 H      -5.264265    -3.262863    -1.698576      27.98
 H      -5.495820    -4.098127    -0.156105      29.13
55
name = lig-etoh-frame_713
 C       1.979195     2.323216    -2.273076      18.04
 H       1.410468     2.907151    -2.832848      14.12
 C       3.227975     1.856389    -0.235358      90.43
 H       3.804811     2.070441     0.586214      18.34
 C       3.657040     0.663840    -0.789469      46.07
 O       4.390740    -0.426947    -0.189145     252.46
 C       5.478808     0.103620     0.773102     111.90
 H       4.952097     0.656124     1.554452      25.46
 H       6.113178     0.583964     0.073725      28.15
 H       5.816451    -0.801542     1.170785      26.98
 C       3.266528     0.336428    -2.060542      38.56
 O       3.915625    -0.925425    -2.611549     197.84
 H       4.122810    -1.569039    -1.755596      21.35
 C       2.431729     1.028960    -2.873049      14.34
 H       2.023276     0.789988    -3.825019      20.62
 C       2.322378     2.652688    -0.992924      85.93
 C       1.641364     3.891833    -0.327231     133.63
 H       1.539822     5.018349    -0.868349      15.44
 O       1.911445     4.102568     1.150925     314.27
 H       2.812240     4.431104     1.109795      30.98
 C      -0.154038     3.798705    -0.325101      63.55
 H      -0.569299     3.470695    -1.276973      16.95
 C      -0.721225     5.248955    -0.001547     111.33
 O       0.053110     6.170457    -0.663765     275.05
 H       0.009857     6.155752    -1.679949      28.09
 H      -0.715931     5.412643     1.121932      24.69
 H      -1.688235     4.936758    -0.244582      25.43
 C      -0.735407    -0.625529    -0.235111      42.03
 H       0.007935    -1.537432    -0.449257      16.79
 C      -3.022483     0.456243    -0.624873      55.41
 H      -4.047737     0.582966    -1.038198      19.51
 C      -2.464079     1.679593    -0.155704     -20.47
 O      -3.161698     2.972335    -0.338356     174.41
 C      -3.805523     3.142058    -1.662564      98.78
 H      -4.560041     2.252605    -2.219168      21.85
 H      -4.161031     4.135697    -1.330390      23.89
 H      -3.125778     3.300131    -2.527936      24.44
 C      -0.979621     1.732709     0.144644       9.74
 O      -0.482175     2.942442     0.690726     200.25
 C      -0.246437     0.636147     0.206888      43.97
 H       0.930266     0.814556     0.323645      13.67
 C      -2.109091    -0.714675    -0.537897      20.45
 C      -2.764879    -1.918509    -1.202395      81.94
 H      -3.253240    -1.471327    -2.024010      21.15
 O      -1.756282    -2.985406    -1.605419     186.45
 H      -2.358995    -3.911960    -1.701428      12.16
 C      -3.778871    -2.552432    -0.219059      80.68
 H      -3.246518    -3.275632     0.548579      16.64
 O      -4.732843    -1.677353     0.564553     294.70
 H      -4.531558    -1.576051     1.723537      21.45
 C      -4.794318    -3.594850    -0.862199      76.93
 O      -3.868905    -4.766585    -1.355825     230.70
 H      -3.422281    -5.300519    -0.516138      24.62
 H      -5.456628    -3.403421    -1.750047      25.42
 H      -5.779743    -3.926781    -0.263447      25.14
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name = lig-etoh-frame_714
 C       1.941156     2.249524    -2.254624      76.59
 H       1.238229     2.990720    -2.924422      25.57
 C       3.236474     1.847692    -0.223070     136.95
 H       3.589424     2.148961     0.861999      21.98
 C       3.690288     0.655480    -0.832737      42.31
 O       4.375095    -0.449330    -0.172221     255.30
 C       5.478701     0.093496     0.816593      80.00
 H       4.779445     0.791308     1.335912      23.75
 H       6.311778     0.651077     0.255369      27.82
 H       6.012393    -0.929634     1.155936      24.03
 C       3.315778     0.250031    -2.114830      10.15
 O       3.906514    -0.871805    -2.550896     156.26
 H       4.150316    -1.354486    -1.570511      18.50
 C       2.435213     1.053569    -2.825373      35.90
 H       2.156607     0.705666    -3.913293      18.39
 C       2.278284     2.750962    -1.010427     104.90
 C       1.594929     3.897178    -0.387880     110.55
 H       1.725684     4.847212    -0.679076      12.34
 O       1.888788     4.147562     1.130745     278.83
 H       2.822285     4.610606     1.252463      27.80
 C      -0.108265     3.819423    -0.335741      54.95
 H      -0.511290     3.632628    -1.373513      16.98
 C      -0.713564     5.238116     0.040253     101.59
 O       0.061257     6.162323    -0.664182     271.56
 H       0.066009     5.972922    -1.608898      30.66
 H      -0.749874     5.572960     1.071729      24.19
 H      -1.775811     4.846071    -0.349221      21.79
 C      -0.696885    -0.640069    -0.247040      56.12
 H      -0.089347    -1.385955    -0.532963      19.99
 C      -2.994077     0.374339    -0.643323      55.13
 H      -4.135302     0.460697    -0.672938      20.38
 C      -2.399357     1.802554    -0.237264     -14.43
 O      -3.144032     2.937053    -0.332076     235.73
 C      -3.715035     3.048659    -1.635409     124.87
 H      -4.612474     2.578787    -1.748964      25.40
 H      -4.503766     3.860602    -1.240532      22.34
 H      -2.963646     3.244415    -2.440314      24.40
 C      -1.058114     1.773750     0.172471      14.75
 O      -0.510678     2.921255     0.720639     214.57
 C      -0.273271     0.607303     0.150252      41.42
 H       0.734626     0.667420     0.433127      17.59
 C      -2.100439    -0.759842    -0.498309      26.34
 C      -2.798190    -1.824121    -1.183485      66.03
 H      -3.286072    -1.504110    -2.199464      19.13
 O      -1.776609    -2.980595    -1.598572     188.04
 H      -2.502282    -3.722075    -1.652018      14.78
 C      -3.847115    -2.580990    -0.154136      74.45
 H      -3.043281    -2.842727     0.573257      18.50
 O      -4.764098    -1.695003     0.617797     360.37
 H      -4.261611    -1.714609     1.410616      27.82
 C      -4.793134    -3.579595    -0.944974      74.28
 O      -3.899876    -4.747235    -1.311363     322.09
 H      -3.334946    -5.200185    -0.671002      28.42
 H      -5.267438    -3.341834    -1.895340      26.80
 H      -5.496217    -3.756431    -0.125139      24.65
55
name = lig-etoh-frame_715
 C       1.876374     2.209110    -2.285602      70.36
 H       1.227768     2.739827    -2.847112      27.00
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 C       3.222666     1.870971    -0.215675      79.51
 H       3.175950     2.189587     0.786710      19.20
 C       3.717636     0.650819    -0.820748      46.46
 O       4.385236    -0.435599    -0.138221     277.98
 C       5.461050     0.054254     0.805115     123.54
 H       4.994648     0.763615     1.502587      29.30
 H       6.284739     0.684237     0.463950      29.59
 H       5.891540    -0.704667     1.336349      29.45
 C       3.354796     0.200073    -2.164058       9.84
 O       3.890103    -0.862934    -2.503208     175.25
 H       4.356881    -1.137676    -1.661782      17.79
 C       2.431847     1.077548    -2.819496      60.85
 H       2.281541     0.766025    -3.773388      22.83
 C       2.296891     2.775744    -0.972497      81.03
 C       1.504800     3.921196    -0.360669     102.13
 H       2.056919     4.930519    -0.927792      12.45
 O       1.864749     4.185454     1.080687     285.50
 H       2.756348     4.521900     1.286758      30.70
 C       0.004777     3.874520    -0.317303      56.37
 H      -0.352613     3.605867    -1.313507      19.30
 C      -0.723257     5.159435     0.055930     109.43
 O       0.065179     6.204966    -0.682220     199.67
 H       0.060509     5.736670    -1.655662      27.22
 H      -0.730834     5.564135     1.079747      24.23
 H      -1.693104     5.343110    -0.350735      25.48
 C      -0.726183    -0.648229    -0.270788      42.90
 H       0.028760    -1.524336    -0.541396      16.36
 C      -2.906680     0.410696    -0.580223      44.78
 H      -3.936917     0.093565    -0.500482      17.17
 C      -2.353689     1.779621    -0.342765      28.36
 O      -3.110927     2.888338    -0.316160     258.44
 C      -3.701390     3.035020    -1.571312     111.95
 H      -4.609093     2.187644    -1.554077      22.48
 H      -4.413349     3.960706    -1.628177      24.74
 H      -2.957673     3.171897    -2.350103      25.07
 C      -1.151697     1.808683     0.224548       7.12
 O      -0.538013     2.902971     0.735143     211.67
 C      -0.272624     0.577933     0.109649      32.17
 H       0.776322     0.676475     0.547132      14.07
 C      -2.124219    -0.737892    -0.513029      32.30
 C      -2.832470    -1.832537    -1.187028      77.69
 H      -3.262036    -1.614377    -2.109693      20.56
 O      -1.831498    -2.943008    -1.578980     246.03
 H      -2.457760    -3.661782    -1.726597      18.10
 C      -3.919542    -2.551230    -0.132816      72.59
 H      -3.083459    -2.904557     0.529115      18.22
 O      -4.773394    -1.722642     0.643030     381.19
 H      -4.248085    -1.684735     1.496707      26.16
 C      -4.719822    -3.599289    -0.959507      68.75
 O      -3.949220    -4.727382    -1.295627     344.72
 H      -3.400000    -5.050651    -0.498967      27.06
 H      -4.970102    -3.134379    -1.940447      26.49
 H      -5.430887    -3.849539    -0.100429      22.87
55
name = lig-etoh-frame_716
 C       1.840952     2.216487    -2.254155     133.97
 H       1.007283     2.691760    -2.966784      19.80
 C       3.164396     1.906436    -0.246462     155.19
 H       3.071688     2.100529     0.875994      13.96
 C       3.712350     0.673641    -0.788290      90.82
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 O       4.423292    -0.391441    -0.085892     286.66
 C       5.420490     0.045155     0.804221     115.57
 H       5.126567     0.644416     1.730557      28.73
 H       6.229003     0.634011     0.291696      26.93
 H       5.754393    -0.828687     1.581017      25.21
 C       3.345573     0.318139    -2.102047      32.73
 O       3.892565    -0.957886    -2.505061      24.89
 H       4.873618    -1.038284    -1.918835      19.11
 C       2.457957     1.054011    -2.837003      44.23
 H       2.172001     0.826279    -3.972266      19.48
 C       2.314451     2.690660    -0.966399     116.51
 C       1.518455     4.005719    -0.293616     115.55
 H       1.846734     4.582225    -1.057311      19.82
 O       1.824456     4.214853     1.028243     264.09
 H       2.827744     4.335718     1.112169      32.35
 C       0.063357     3.913316    -0.286516      57.78
 H      -0.231477     3.461455    -1.245395      20.37
 C      -0.695466     5.144651     0.048348     101.51
 O       0.061831     6.247405    -0.720304     199.06
 H       0.112244     5.936934    -1.615634      31.75
 H      -0.628948     5.304906     1.160306      24.57
 H      -1.672594     5.480976    -0.409309      23.48
 C      -0.754083    -0.683738    -0.316676      40.25
 H      -0.095227    -1.498621    -0.346762      16.42
 C      -2.824665     0.481406    -0.485339      54.64
 H      -3.876518     0.059484    -0.549132      14.69
 C      -2.360992     1.669361    -0.422818      31.68
 O      -3.085537     2.873530    -0.290000     268.11
 C      -3.800210     3.027553    -1.517996     120.72
 H      -4.095276     2.049945    -1.778633      24.91
 H      -4.013441     4.072433    -1.938267      23.89
 H      -3.006767     2.873289    -2.380321      24.40
 C      -1.121138     1.757975     0.270596      -3.63
 O      -0.547659     2.912105     0.740526     185.30
 C      -0.271488     0.602608     0.114870      24.31
 H       0.772179     0.770620     0.519934      10.70
 C      -2.125014    -0.689574    -0.577631      31.55
 C      -2.862019    -1.923561    -1.167515      66.92
 H      -3.413902    -1.536750    -2.147659      18.05
 O      -1.899926    -2.877402    -1.544536     211.95
 H      -2.361892    -3.830490    -1.953037      13.22
 C      -3.921196    -2.505253    -0.146142      74.19
 H      -3.346443    -3.308661     0.485708      17.82
 O      -4.772871    -1.749921     0.658833     375.21
 H      -4.587366    -1.506122     1.750416      23.65
 C      -4.646884    -3.596294    -0.904209      94.71
 O      -3.971248    -4.738026    -1.290716     284.24
 H      -3.591298    -4.978753    -0.342884      25.96
 H      -4.911848    -3.045580    -1.802556      26.65
 H      -5.691083    -3.978363    -0.538395      24.07
55
name = lig-etoh-frame_717
 C       1.830188     2.222570    -2.239249      88.09
 H       1.027895     2.699586    -2.783929      19.53
 C       3.128603     1.891392    -0.229415     113.05
 H       3.285944     1.970166     0.844923      13.87
 C       3.690143     0.717274    -0.728492      49.33
 O       4.439770    -0.323405    -0.040637     278.35
 C       5.410786     0.042382     0.884447     117.27
 H       5.029833     0.722649     1.653813      29.34
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 H       6.196986     0.402467     0.188869      25.36
 H       5.683798    -0.912707     1.213839      27.45
 C       3.380774     0.382971    -2.019982      92.44
 O       3.913560    -1.033771    -2.510082     221.37
 H       4.799872    -1.132977    -2.470268      23.18
 C       2.449062     1.063769    -2.888246     -33.30
 H       2.146204     0.807139    -3.836058      16.17
 C       2.241586     2.616700    -0.995853      61.33
 C       1.574743     4.002440    -0.260051     105.85
 H       1.704612     4.841744    -1.213214      15.93
 O       1.828984     4.265871     1.009245     254.44
 H       2.859036     4.135311     1.068443      28.31
 C       0.024150     3.879478    -0.288470      71.75
 H      -0.210069     3.418234    -1.263227      18.25
 C      -0.643282     5.211571     0.006262     104.20
 O       0.061953     6.304653    -0.729634     220.21
 H       0.067679     6.102917    -1.759230      27.01
 H      -0.553223     5.199163     1.084146      25.74
 H      -1.693270     5.042598    -0.307649      24.79
 C      -0.765794    -0.669684    -0.341319      47.49
 H      -0.160315    -1.624874    -0.244139      16.03
 C      -2.880284     0.423865    -0.437388      45.85
 H      -3.942026     0.548224    -0.671138      16.50
 C      -2.319051     1.694507    -0.387359      14.39
 O      -3.076144     2.871596    -0.271967     242.33
 C      -3.830578     3.005815    -1.548065     114.89
 H      -4.320749     2.049553    -2.032158      23.71
 H      -4.038949     3.999238    -1.805466      26.44
 H      -2.966926     2.738849    -2.278995      23.55
 C      -1.017545     1.680866     0.260508       5.55
 O      -0.543654     2.936621     0.749696     200.08
 C      -0.263286     0.617366     0.152046      50.48
 H       0.746028     0.750302     0.422434      12.95
 C      -2.086348    -0.705639    -0.667524      29.73
 C      -2.910202    -1.966038    -1.138935      89.69
 H      -3.511157    -1.560315    -1.900264      20.28
 O      -1.950939    -2.847998    -1.530643     320.29
 H      -2.276350    -3.578436    -1.915488      22.29
 C      -3.874015    -2.549794    -0.102525      92.86
 H      -3.401134    -3.288592     0.557060      19.56
 O      -4.795731    -1.742503     0.680500     438.67
 H      -4.708743    -1.704954     1.562887      35.26
 C      -4.700325    -3.554858    -0.898666      90.89
 O      -3.955276    -4.773637    -1.267504     327.29
 H      -3.626122    -5.242290    -0.522025      32.18
 H      -4.971079    -3.109320    -1.886683      26.52
 H      -5.731434    -3.826863    -0.719761      24.56
55
name = lig-etoh-frame_718
 C       1.838803     2.190000    -2.273933      12.53
 H       1.025257     2.841362    -2.708276      18.15
 C       3.119646     1.847633    -0.166919      45.15
 H       3.456286     2.116302     0.852619      15.98
 C       3.692423     0.723104    -0.660755      50.97
 O       4.395043    -0.241420    -0.024537     251.50
 C       5.426719     0.046047     0.949532     110.61
 H       5.062095     0.845249     1.635641      25.94
 H       6.356721     0.388677     0.423329      26.31
 H       5.772899    -1.069381     1.126340      24.28
 C       3.434087     0.344072    -2.039391      68.38
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 O       3.882397    -1.052002    -2.516458     130.41
 H       4.925667    -1.208619    -2.846882      18.71
 C       2.450548     1.099526    -2.860494      60.69
 H       2.152644     0.632283    -3.881580      20.68
 C       2.135353     2.622921    -0.962030      78.51
 C       1.576763     3.941542    -0.370699     113.62
 H       1.725685     4.885787    -0.755769      20.12
 O       1.893632     4.322281     1.034558     296.38
 H       2.819919     4.223685     1.286861      30.41
 C      -0.016666     3.804332    -0.319924      87.65
 H      -0.346214     3.499573    -1.316567      19.72
 C      -0.592963     5.266177    -0.069814     101.83
 O       0.046854     6.363522    -0.727255     234.18
 H      -0.146344     6.141719    -1.725502      28.04
 H      -0.487212     5.501586     1.043415      24.91
 H      -1.640249     4.835412    -0.146262      23.03
 C      -0.736740    -0.634068    -0.337007      51.02
 H      -0.218127    -1.624927    -0.283355      16.59
 C      -2.986831     0.392145    -0.454975      32.47
 H      -3.992266     0.729500    -0.753002      13.19
 C      -2.252773     1.734145    -0.245330       3.40
 O      -3.091294     2.863203    -0.275184     189.43
 C      -3.794333     2.929310    -1.634293      97.69
 H      -4.857289     2.469884    -1.769764      23.15
 H      -4.350773     4.008732    -1.520956      23.27
 H      -2.905653     2.935904    -2.279794      22.69
 C      -0.959039     1.721443     0.210974       6.24
 O      -0.526553     2.957762     0.753655     231.95
 C      -0.205441     0.528406     0.187952      39.70
 H       0.966108     0.606009     0.409534      13.00
 C      -2.112033    -0.754857    -0.742736      23.16
 C      -2.944216    -1.921952    -1.066202      69.62
 H      -3.714782    -1.601290    -1.908414      17.79
 O      -1.953492    -2.839901    -1.536532     247.58
 H      -2.468261    -3.693741    -1.952491      14.74
 C      -3.864484    -2.647577    -0.008693      62.16
 H      -3.129500    -3.096499     0.810576      17.89
 O      -4.823066    -1.719135     0.651124     294.52
 H      -4.602174    -2.000471     1.755669      19.77
 C      -4.787890    -3.534089    -0.958701      46.62
 O      -3.941757    -4.806077    -1.257977     257.19
 H      -3.586508    -5.526484    -0.576487      26.30
 H      -4.835988    -3.211403    -2.014257      26.93
 H      -5.844168    -3.663923    -0.346512      23.72
55
name = lig-etoh-frame_719
 C       1.827255     2.189479    -2.289865      37.94
 H       1.112640     2.889614    -2.887401      19.46
 C       3.075804     1.860692    -0.095713      13.87
 H       3.473277     2.406268     0.801710      20.44
 C       3.693183     0.688676    -0.680247      52.54
 O       4.362079    -0.180795     0.008770     221.24
 C       5.465953     0.035474     0.974856     119.03
 H       5.224852     0.708363     1.834212      24.65
 H       6.415995     0.550125     0.675206      26.21
 H       5.682063    -0.888098     1.488381      26.77
 C       3.470014     0.272993    -2.108541      44.23
 O       3.833879    -1.027179    -2.520041     189.19
 H       4.778001    -1.048791    -2.961287      22.34
 C       2.498500     1.068947    -2.809948      42.27
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 H       2.232454     0.607295    -3.772789      21.49
 C       2.105227     2.626549    -0.884273      70.17
 C       1.538005     3.856035    -0.440618      97.64
 H       1.906209     4.929289    -0.842355      20.60
 O       1.939900     4.357976     1.068888     232.75
 H       2.971791     4.409909     1.303287      26.56
 C      -0.009414     3.785400    -0.357228      83.43
 H      -0.537538     3.516092    -1.315923      18.53
 C      -0.556819     5.269321    -0.077558     103.64
 O       0.001404     6.409126    -0.755289     220.04
 H      -0.169149     6.251527    -1.662313      32.92
 H      -0.403640     5.708524     0.876169      25.38
 H      -1.682988     5.283679    -0.214219      25.18
 C      -0.738410    -0.645830    -0.336170      38.73
 H      -0.142415    -1.529891    -0.402995      18.31
 C      -2.994509     0.451657    -0.510463      23.47
 H      -4.081013     0.411744    -0.794468      15.98
 C      -2.279563     1.677339    -0.093832      -7.28
 O      -3.113693     2.846293    -0.297732     177.57
 C      -3.799106     2.926719    -1.667106     116.92
 H      -4.820321     2.587499    -1.485435      23.09
 H      -4.194863     3.866932    -1.412970      25.83
 H      -3.123026     3.033264    -2.562152      24.29
 C      -0.908585     1.789534     0.180671       9.66
 O      -0.490091     2.977322     0.735808     251.55
 C      -0.102704     0.448782     0.220516      24.74
 H       0.867477     0.410388     0.453525      18.42
 C      -2.204482    -0.707492    -0.746698      22.96
 C      -2.974123    -1.888887    -1.020318      81.04
 H      -3.654093    -1.689833    -1.786263      20.06
 O      -1.953524    -2.870529    -1.576245     244.77
 H      -2.596602    -3.711717    -1.741327      13.91
 C      -3.877468    -2.705441     0.070885      80.59
 H      -3.171950    -3.056067     0.763393      21.81
 O      -4.819884    -1.718261     0.647790     362.78
 H      -4.783033    -1.892525     1.610227      25.32
 C      -4.830638    -3.582700    -0.949877      69.04
 O      -3.951045    -4.842906    -1.272362     263.77
 H      -3.682089    -5.355512    -0.442724      27.68
 H      -4.841527    -3.169844    -1.956968      29.12
 H      -5.651399    -3.627024    -0.328905      25.95
55
name = lig-etoh-frame_720
 C       1.833603     2.207981    -2.253508      87.58
 H       1.286746     2.718565    -3.011210      23.35
 C       3.022568     1.897508    -0.078898       6.54
 H       3.384068     2.378345     0.778737      22.46
 C       3.658874     0.700964    -0.763059      57.80
 O       4.392740    -0.177622     0.090064     210.38
 C       5.493125     0.059069     1.031090     111.43
 H       5.143219     0.596772     1.947111      22.85
 H       6.363565     0.567968     0.599180      24.83
 H       5.610230    -0.883832     1.671614      23.66
 C       3.469429     0.242908    -2.113507      37.90
 O       3.783818    -0.987710    -2.534586     249.55
 H       4.599655    -0.936117    -2.888646      27.30
 C       2.551911     1.013440    -2.767698      51.44
 H       2.258462     0.700687    -3.784062      20.05
 C       2.146683     2.560182    -0.864967      72.02
 C       1.504848     3.864267    -0.426993      94.87
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 H       1.920038     4.481852    -1.244321      23.38
 O       1.967324     4.372265     1.091476     255.93
 H       2.932909     4.497065     0.936489      29.01
 C      -0.003591     3.863120    -0.395838      90.04
 H      -0.498457     3.455680    -1.259096      20.87
 C      -0.560894     5.286756    -0.056566      96.11
 O      -0.037064     6.453543    -0.809260     168.33
 H      -0.085654     6.335582    -1.879181      27.12
 H      -0.304630     5.536937     1.034155      24.53
 H      -1.579198     5.598661    -0.316064      23.73
 C      -0.794653    -0.680851    -0.342453      23.01
 H      -0.076629    -1.575600    -0.598288      16.78
 C      -2.943807     0.521008    -0.573569      73.35
 H      -3.966247     0.221366    -0.698800      19.48
 C      -2.375769     1.606162    -0.001298      -5.86
 O      -3.111819     2.818642    -0.329902     179.49
 C      -3.817461     2.980803    -1.619937      87.20
 H      -4.639458     2.146963    -1.583130      22.28
 H      -3.910116     4.178461    -1.542303      23.02
 H      -3.549987     2.824301    -2.749607      24.36
 C      -0.865832     1.754827     0.197294      -9.67
 O      -0.436721     2.998285     0.701050     207.44
 C      -0.084039     0.451221     0.225186       5.91
 H       1.063934     0.278372     0.608772      15.68
 C      -2.249770    -0.595825    -0.671976      26.02
 C      -2.969095    -1.931955    -0.999176      60.18
 H      -3.727511    -1.646508    -1.855797      18.74
 O      -1.983847    -2.909271    -1.611581     263.82
 H      -2.457620    -3.717389    -1.602379      18.21
 C      -3.920650    -2.680140     0.069336      71.87
 H      -3.267670    -3.369042     0.849123      18.07
 O      -4.807339    -1.730201     0.638811     356.24
 H      -4.937176    -1.722577     1.706356      25.19
 C      -4.755716    -3.669513    -0.887239      71.35
 O      -3.998515    -4.865442    -1.284722     316.55
 H      -3.734024    -5.098294    -0.392755      30.53
 H      -5.052522    -3.039084    -1.772305      27.14
 H      -5.900833    -3.901640    -0.379430      25.20
55
name = lig-etoh-frame_721
 C       1.912308     2.151354    -2.198386      84.23
 H       1.296489     2.701628    -3.075108      18.34
 C       3.028977     1.856997    -0.126833      43.06
 H       3.310782     2.137175     0.960229      17.71
 C       3.657095     0.736583    -0.757966      87.01
 O       4.431922    -0.200287     0.162465     209.61
 C       5.478083     0.098613     1.125731     105.18
 H       5.019123     0.800337     1.870775      22.52
 H       6.333042     0.460762     0.509488      22.71
 H       5.739166    -0.974808     1.394751      22.74
 C       3.431241     0.266504    -2.028772      64.39
 O       3.739403    -0.977901    -2.561665     116.17
 H       4.823706    -1.014490    -2.875665      19.08
 C       2.534267     1.026777    -2.760749      74.91
 H       2.291724     0.820366    -3.875591      21.59
 C       2.139534     2.531244    -0.902999      74.09
 C       1.505361     3.893337    -0.378155     104.35
 H       1.827939     4.413288    -1.391849      22.19
 O       1.973571     4.369977     1.043676     261.59
 H       2.910305     4.536409     0.772838      29.75
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 C      -0.018776     3.973441    -0.422900      89.01
 H      -0.329677     3.480447    -1.393727      19.11
 C      -0.571277     5.346421    -0.038508      98.57
 O      -0.043004     6.507010    -0.882143     215.50
 H      -0.009408     6.158977    -1.796919      30.81
 H      -0.311060     5.285803     0.989631      25.56
 H      -1.723817     5.351924    -0.191574      23.35
 C      -0.842531    -0.687989    -0.343187      50.51
 H      -0.373310    -1.547199    -0.642264      19.31
 C      -2.936431     0.555197    -0.616296      80.86
 H      -4.067751     0.446065    -0.631841      22.49
 C      -2.412947     1.634528     0.025239      -9.75
 O      -3.077955     2.801114    -0.353522     215.09
 C      -3.866252     3.031426    -1.563261     112.52
 H      -4.575569     2.255579    -1.661409      25.20
 H      -4.006010     4.030453    -1.739158      26.53
 H      -3.418487     2.579453    -2.540105      25.64
 C      -0.873264     1.653334     0.259640      -9.39
 O      -0.384001     2.998489     0.662294     176.30
 C      -0.118481     0.478658     0.211773      40.23
 H       0.827687     0.377024     0.545252      18.49
 C      -2.176650    -0.619270    -0.582286      21.09
 C      -2.954153    -1.981846    -1.018104      66.28
 H      -3.635813    -1.642740    -1.750868      20.53
 O      -2.025684    -2.914958    -1.634105     230.63
 H      -2.358646    -3.987875    -1.510421      11.69
 C      -3.948478    -2.676589     0.055008      87.03
 H      -3.546357    -3.337312     0.734343      21.39
 O      -4.801582    -1.738422     0.628933     379.58
 H      -4.891320    -1.676834     1.746079      25.22
 C      -4.733826    -3.739663    -0.803875     112.80
 O      -4.065133    -4.867093    -1.287638     307.97
 H      -3.519547    -5.196635    -0.394272      27.57
 H      -5.155647    -3.142684    -1.585208      28.75
 H      -5.610112    -4.167117    -0.483403      26.71
55
name = lig-etoh-frame_722
 C       1.969989     2.101502    -2.215533      50.66
 H       1.343733     2.717837    -2.718559      18.80
 C       3.078199     1.782907    -0.158414     105.29
 H       3.134939     1.848578     0.886495      15.24
 C       3.725597     0.727665    -0.634233      46.68
 O       4.436230    -0.226363     0.190694     244.85
 C       5.446657     0.139968     1.174772     124.10
 H       5.175796     0.933240     1.880577      26.55
 H       6.343563     0.519270     0.642911      25.93
 H       5.841369    -0.865239     1.379708      24.53
 C       3.373564     0.281466    -1.959475      61.67
 O       3.738516    -0.975277    -2.601632     177.38
 H       4.697172    -1.213812    -2.551204      24.57
 C       2.499324     1.056207    -2.793315      26.14
 H       2.379686     0.836095    -3.777733      23.62
 C       2.095553     2.573959    -0.899785      89.34
 C       1.527697     3.923852    -0.355850     106.62
 H       1.807731     4.789990    -1.043413      20.79
 O       1.965853     4.355248     0.921134     249.66
 H       2.992329     4.541657     0.996713      30.09
 C      -0.016770     4.022286    -0.454804      79.01
 H      -0.229615     3.733766    -1.474889      19.54
 C      -0.611059     5.401571    -0.056022     102.02
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 O      -0.047368     6.533925    -0.924305     211.71
 H       0.022577     5.975691    -1.797544      29.18
 H      -0.301971     5.487685     1.048798      24.06
 H      -1.663131     5.096731     0.020705      24.22
 C      -0.838176    -0.655936    -0.312566      56.39
 H      -0.448608    -1.753156    -0.553483      15.67
 C      -2.968753     0.529191    -0.602713      81.60
 H      -4.010121     0.713940    -0.763064      24.82
 C      -2.375998     1.704356    -0.035664      -9.42
 O      -3.035629     2.843447    -0.345470     199.04
 C      -3.875130     2.992185    -1.539464      82.62
 H      -5.042791     2.571868    -1.498146      22.29
 H      -4.285704     4.094344    -1.804706      22.78
 H      -2.980752     2.590436    -2.099492      21.85
 C      -0.948313     1.627019     0.341094       1.12
 O      -0.350419     2.965422     0.626362     165.00
 C      -0.216789     0.487086     0.173407      49.36
 H       0.921413     0.532347     0.471433      13.23
 C      -2.159279    -0.736890    -0.529964      21.49
 C      -2.926735    -2.011621    -1.016940      68.53
 H      -3.665036    -1.603550    -1.829945      19.57
 O      -2.060152    -2.934990    -1.649005     301.01
 H      -2.338275    -3.806023    -1.535031      19.00
 C      -3.962943    -2.702662     0.020701      75.79
 H      -3.401883    -3.286731     0.960554      17.05
 O      -4.816514    -1.723579     0.628505     417.31
 H      -4.654582    -1.836458     1.521085      30.05
 C      -4.771146    -3.759648    -0.736137      74.17
 O      -4.073742    -4.892938    -1.277523     357.94
 H      -3.494099    -5.435103    -0.789969      31.91
 H      -5.206214    -3.300588    -1.690872      25.99
 H      -5.631356    -4.364288    -0.007441      22.51
55
name = lig-etoh-frame_723
 C       1.948459     2.175316    -2.208016      39.74
 H       1.146604     2.912274    -2.730511      15.42
 C       3.068659     1.782504    -0.142682     118.00
 H       3.030763     1.829051     1.001783      14.39
 C       3.816515     0.626588    -0.553552      28.23
 O       4.426780    -0.249716     0.205897     275.16
 C       5.440909     0.187971     1.168392     120.04
 H       5.243577     0.876226     2.045432      25.42
 H       6.313736     0.728873     0.725499      26.78
 H       5.823698    -0.733846     1.803745      24.38
 C       3.339914     0.253477    -1.936737      51.87
 O       3.740385    -0.956897    -2.618214     154.70
 H       4.595521    -1.339857    -2.170752      25.50
 C       2.532174     1.008755    -2.804707      33.33
 H       2.405367     0.690511    -3.957499      19.70
 C       2.118424     2.598686    -0.859913      63.34
 C       1.563311     3.983295    -0.380803     102.93
 H       1.939175     5.009634    -0.909997      18.12
 O       1.961732     4.338605     0.828425     284.85
 H       2.885698     4.324650     1.088876      31.51
 C       0.025624     4.023012    -0.457785      59.16
 H      -0.343448     3.871866    -1.505474      17.77
 C      -0.620603     5.432514    -0.043434      97.32
 O      -0.079379     6.514936    -0.942800     164.70
 H       0.037709     6.079174    -1.919100      27.98
 H      -0.291134     5.913275     0.858141      23.87
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 H      -1.765116     5.213013     0.010554      23.83
 C      -0.802278    -0.704354    -0.275433      47.34
 H      -0.223532    -1.571905    -0.254179      17.84
 C      -2.956368     0.476322    -0.526472      23.30
 H      -3.966128     0.639787    -1.039024      14.89
 C      -2.324286     1.706864    -0.161727      15.39
 O      -3.009093     2.954271    -0.287135     225.45
 C      -3.897374     2.948940    -1.519079     122.08
 H      -4.875885     2.663928    -1.346686      26.69
 H      -4.037739     3.982053    -1.632334      27.07
 H      -3.143877     2.632078    -2.233096      24.65
 C      -1.064051     1.718655     0.395347      -4.79
 O      -0.339132     2.913571     0.590847     187.48
 C      -0.269838     0.495692     0.158869      33.07
 H       0.806005     0.669443     0.229942      12.87
 C      -2.269760    -0.811133    -0.519302      12.92
 C      -2.939783    -2.018003    -1.015990      78.12
 H      -3.584890    -1.632512    -1.783186      18.76
 O      -2.062220    -2.942447    -1.667801     274.12
 H      -2.538309    -3.863163    -1.579684      13.09
 C      -3.931635    -2.743612     0.014155      94.65
 H      -3.304534    -3.062241     0.749377      20.45
 O      -4.838355    -1.707550     0.608116     372.24
 H      -4.433313    -1.904739     1.668952      19.28
 C      -4.858597    -3.816119    -0.643465      82.69
 O      -4.059587    -4.929696    -1.308135     321.26
 H      -3.502112    -5.605857    -0.754411      27.69
 H      -5.348566    -3.502449    -1.539931      28.61
 H      -5.450231    -4.003946     0.174601      26.30
55
name = lig-etoh-frame_724
 C       1.883024     2.290605    -2.215450      71.91
 H       1.268955     2.776952    -2.868358      23.12
 C       3.048386     1.788237    -0.060556      57.68
 H       3.074193     2.042201     0.990487      16.17
 C       3.791070     0.582783    -0.592561      20.13
 O       4.452649    -0.303012     0.260283     272.58
 C       5.465003     0.234921     1.202061     116.24
 H       4.915529     0.824453     1.966262      24.25
 H       6.225411     0.800572     0.641657      26.39
 H       5.728242    -0.550943     1.840025      25.58
 C       3.358714     0.185026    -1.930993      23.10
 O       3.770611    -0.933035    -2.612390     177.73
 H       4.238594    -1.487744    -1.763611      23.07
 C       2.555853     0.992366    -2.790934      36.42
 H       2.412077     0.636260    -3.727978      17.68
 C       2.196976     2.601892    -0.860462      22.99
 C       1.605712     4.049083    -0.483481      99.99
 H       2.005921     4.746990    -1.256022      21.52
 O       1.945927     4.330755     0.848816     289.49
 H       2.972476     4.069669     0.917919      24.62
 C       0.054679     4.019487    -0.428638      48.24
 H      -0.475487     3.761723    -1.352359      19.57
 C      -0.610590     5.458137    -0.036437     100.74
 O      -0.124647     6.479436    -0.966185     196.41
 H      -0.083193     6.221490    -1.914415      30.28
 H      -0.299465     6.049437     0.869944      22.87
 H      -1.677500     5.521103    -0.173986      25.59
 C      -0.827957    -0.766012    -0.218345      24.58
 H       0.067114    -1.511030    -0.093108      15.29
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 C      -2.942065     0.414905    -0.466034      55.86
 H      -3.783882     0.322514    -1.105701      16.74
 C      -2.323822     1.701386    -0.273239      21.05
 O      -2.993162     3.043579    -0.236870     200.66
 C      -3.860589     2.958456    -1.471997      97.99
 H      -4.867197     2.290115    -1.208084      23.24
 H      -3.800238     4.109970    -1.574638      23.54
 H      -3.695834     2.521976    -2.605737      24.00
 C      -1.114289     1.802051     0.383125      -4.54
 O      -0.333512     2.880931     0.560990     181.87
 C      -0.330086     0.547503     0.162049      -3.72
 H       0.760599     0.694473     0.122994      12.95
 C      -2.324505    -0.806375    -0.500847      22.47
 C      -3.001080    -2.032651    -1.032885      68.92
 H      -3.704166    -1.637198    -1.865809      18.46
 O      -2.046579    -2.967889    -1.674835     231.32
 H      -2.759864    -3.790488    -1.812803      13.27
 C      -3.906242    -2.734953    -0.031651      84.74
 H      -3.075230    -3.181114     0.772486      16.31
 O      -4.823911    -1.726301     0.614941     386.69
 H      -4.747801    -1.556718     1.540664      29.08
 C      -4.881482    -3.881026    -0.561960      62.45
 O      -4.046496    -4.975614    -1.336612     271.40
 H      -3.720216    -5.442786    -0.474344      25.06
 H      -5.655730    -3.505813    -1.314464      27.97
 H      -5.590976    -3.962902     0.484661      25.11
55
name = lig-etoh-frame_725
 C       1.901065     2.279394    -2.244118      66.68
 H       1.276644     2.843567    -3.068202      22.36
 C       3.045367     1.768490    -0.005141      56.18
 H       3.258971     2.202186     0.996698      20.59
 C       3.681060     0.603632    -0.630927       7.31
 O       4.488774    -0.371495     0.306886     212.40
 C       5.438130     0.304436     1.241487      92.13
 H       4.681730     0.964428     1.715069      21.68
 H       6.203031     0.819670     0.648079      25.18
 H       5.909222    -0.678545     1.783175      22.33
 C       3.378029     0.158548    -1.936236      14.90
 O       3.824782    -0.950192    -2.556467     259.81
 H       3.961522    -1.550524    -1.931670      30.08
 C       2.539586     1.067405    -2.688336      48.74
 H       2.308269     0.582481    -3.755342      16.90
 C       2.263321     2.631614    -0.910130      39.55
 C       1.632685     4.042467    -0.578136      82.72
 H       2.009087     4.622781    -1.549346      19.73
 O       1.951719     4.330366     0.895903     306.88
 H       2.907579     4.156457     0.865910      26.47
 C       0.028801     4.016770    -0.388182      51.56
 H      -0.472179     3.630329    -1.281448      20.00
 C      -0.572949     5.493764    -0.046624      96.39
 O      -0.149830     6.471191    -0.976889     218.29
 H      -0.287633     6.080046    -2.013009      23.84
 H      -0.375116     5.733035     1.014238      24.59
 H      -1.723535     5.545065    -0.247239      23.24
 C      -0.878595    -0.766187    -0.124588      38.04
 H      -0.092447    -1.513698    -0.197165      17.43
 C      -2.952167     0.391573    -0.453738      45.77
 H      -3.908511     0.212341    -1.022110      15.35
 C      -2.364276     1.732880    -0.303703      26.44
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 O      -2.976901     3.049476    -0.254399     254.28
 C      -3.864996     3.001622    -1.426489     136.91
 H      -4.635484     2.452212    -1.087434      29.54
 H      -4.164206     4.046297    -1.665410      27.13
 H      -3.803860     2.491836    -2.327238      29.15
 C      -1.089991     1.796541     0.283633       2.82
 O      -0.308553     2.902114     0.554680     191.70
 C      -0.408065     0.583224     0.171655      17.03
 H       0.762017     0.654864     0.191610      14.48
 C      -2.249795    -0.820149    -0.463135      25.17
 C      -3.078495    -2.033487    -1.099746      73.60
 H      -3.754339    -1.707158    -1.883087      20.46
 O      -2.060391    -2.998324    -1.675656     286.29
 H      -2.568548    -3.662536    -2.023973      22.63
 C      -3.883185    -2.732508    -0.016188     103.48
 H      -3.288085    -3.244296     0.607464      21.55
 O      -4.807256    -1.755903     0.587569     389.74
 H      -4.849980    -1.498973     1.572098      30.04
 C      -4.901750    -3.907650    -0.478391      93.68
 O      -4.071431    -5.002872    -1.306544     329.07
 H      -3.711403    -5.354413    -0.513028      29.96
 H      -5.737151    -3.500532    -1.019801      29.46
 H      -5.386302    -4.367386     0.325459      29.75
55
name = lig-etoh-frame_726
 C       1.974674     2.211249    -2.278002      37.93
 H       1.418058     2.878268    -2.889102      23.15
 C       3.034492     1.768149    -0.028528      64.91
 H       3.489345     2.174167     0.907628      23.52
 C       3.586902     0.605647    -0.577215      16.57
 O       4.502683    -0.420023     0.303477     184.98
 C       5.377131     0.340396     1.250934     126.04
 H       4.865528     1.139746     1.819092      25.16
 H       6.211837     0.897033     0.740931      26.09
 H       5.912018    -0.360967     1.747444      27.29
 C       3.364066     0.212238    -1.925213       9.95
 O       3.882378    -0.977096    -2.516091     183.99
 H       3.921872    -1.860928    -1.890321      22.46
 C       2.509300     1.100952    -2.625548      50.02
 H       2.212730     0.777886    -3.581685      20.96
 C       2.299381     2.677819    -0.956874      42.59
 C       1.633626     3.976550    -0.599792      88.61
 H       1.890013     4.793478    -1.372990      20.64
 O       1.964058     4.343544     0.895805     286.74
 H       2.981304     4.449963     1.094504      25.02
 C      -0.013914     3.999766    -0.386591      64.92
 H      -0.397945     3.675195    -1.392454      19.56
 C      -0.575390     5.477556    -0.061853     109.86
 O      -0.154554     6.482401    -0.993363     296.38
 H      -0.219615     6.020484    -1.788732      32.94
 H      -0.363025     5.527078     1.013979      24.21
 H      -1.629430     5.254272    -0.061569      25.23
 C      -0.925650    -0.709161    -0.026515      56.28
 H      -0.343342    -1.631995    -0.288484      18.33
 C      -2.989931     0.420367    -0.490601      52.58
 H      -4.063388     0.396507    -0.698115      18.54
 C      -2.417368     1.763363    -0.256311      11.45
 O      -2.954862     3.007307    -0.330769     237.57
 C      -3.929974     3.084642    -1.362860      93.11
 H      -4.946491     2.608958    -0.793304      23.08
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 H      -4.526293     3.991344    -1.694578      23.82
 H      -3.304334     2.385339    -2.199360      22.09
 C      -1.041281     1.762798     0.127624      15.93
 O      -0.277309     2.953842     0.574991     210.16
 C      -0.420242     0.557323     0.194703      56.18
 H       0.573541     0.630625     0.397143      18.72
 C      -2.186872    -0.852103    -0.453462      33.90
 C      -3.094276    -2.044145    -1.153666      58.93
 H      -3.782465    -1.666852    -1.971845      19.37
 O      -2.079087    -2.997940    -1.666422     221.65
 H      -2.496769    -3.800003    -2.330115      17.69
 C      -3.936689    -2.752397     0.019151      72.57
 H      -3.181570    -3.323852     0.820923      15.10
 O      -4.799001    -1.774202     0.538884     329.62
 H      -4.647892    -1.886040     1.654850      22.35
 C      -4.883907    -3.923374    -0.424271      77.60
 O      -4.136143    -4.996412    -1.253260     287.07
 H      -3.401271    -5.498697    -0.624789      22.76
 H      -5.765057    -3.503622    -0.991144      27.06
 H      -5.069054    -4.866034     0.356023      23.20
55
name = lig-etoh-frame_727
 C       2.043743     2.253109    -2.217400      26.39
 H       1.434848     2.897151    -2.877210      19.04
 C       3.027605     1.818082    -0.098107      76.85
 H       3.475903     2.119633     0.808818      20.86
 C       3.544498     0.545856    -0.488031      16.96
 O       4.487570    -0.409748     0.277169     212.90
 C       5.316349     0.396491     1.217391     110.22
 H       5.010628     1.105382     2.038077      25.59
 H       6.090708     0.953841     0.685687      27.19
 H       5.907546    -0.309322     2.049333      26.22
 C       3.351147     0.243899    -1.868947      32.04
 O       3.926941    -0.992741    -2.481731     167.60
 H       3.939738    -1.771635    -1.767568      22.45
 C       2.517178     0.991702    -2.662227      40.27
 H       2.173804     0.766285    -3.710792      23.02
 C       2.322468     2.697726    -0.975123      40.47
 C       1.617429     3.939889    -0.515073     104.05
 H       1.838624     4.948312    -1.097826      17.25
 O       1.986647     4.358853     0.865294     310.36
 H       2.873701     4.748048     1.141672      27.81
 C      -0.005527     3.969620    -0.445961      73.13
 H      -0.382161     3.771306    -1.443406      18.23
 C      -0.586839     5.382732    -0.053728      88.93
 O      -0.160209     6.499994    -0.960691     204.44
 H       0.010409     6.028200    -1.995257      22.52
 H      -0.157022     5.719011     0.948188      22.06
 H      -1.711326     5.091875     0.048305      22.74
 C      -0.946992    -0.707311     0.033479      48.11
 H      -0.388976    -1.688583    -0.131106      17.89
 C      -3.021102     0.479974    -0.527179      82.41
 H      -4.118657     0.526443    -0.437758      24.46
 C      -2.439850     1.734732    -0.187313      -2.56
 O      -2.938610     2.998259    -0.400202     222.53
 C      -4.055168     3.093340    -1.304209     114.17
 H      -4.892604     2.656568    -0.971914      28.54
 H      -4.343399     4.161856    -1.658879      25.08
 H      -3.511919     2.657265    -2.006024      27.70
 C      -0.998557     1.769816    -0.014132      15.86
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 O      -0.278487     2.988442     0.587487     183.82
 C      -0.365561     0.526720     0.240333      33.53
 H       0.743018     0.594954     0.745987      16.46
 C      -2.284715    -0.819765    -0.499021      21.25
 C      -3.054964    -2.083821    -1.156374      66.84
 H      -3.681058    -1.596031    -1.938034      21.56
 O      -2.094709    -3.001196    -1.680400     295.83
 H      -2.526293    -3.614531    -2.304033      23.28
 C      -3.977013    -2.819797     0.046257      97.00
 H      -3.255282    -3.000126     0.741573      22.03
 O      -4.788849    -1.790737     0.546189     423.75
 H      -4.687910    -2.018454     1.398723      30.24
 C      -4.822841    -4.015755    -0.365838     101.19
 O      -4.189584    -4.987712    -1.217744     394.53
 H      -3.382266    -5.348424    -0.856486      31.93
 H      -5.700629    -3.708073    -0.924448      27.27
 H      -5.052182    -4.512742     0.496101      28.31
55
name = lig-etoh-frame_728
 C       2.097550     2.289993    -2.205919      22.82
 H       1.434947     2.830193    -2.945544      17.73
 C       3.063892     1.849681    -0.145601      56.86
 H       3.270247     2.262012     0.921419      16.32
 C       3.531947     0.481430    -0.422115      16.13
 O       4.439990    -0.334626     0.258409     251.95
 C       5.303264     0.427729     1.227167     101.10
 H       4.689607     1.030766     1.941042      26.04
 H       5.977452     0.976785     0.530669      26.27
 H       5.702803    -0.282716     1.817484      28.76
 C       3.358136     0.175894    -1.813898      14.34
 O       3.949007    -0.977785    -2.429084     228.46
 H       4.063307    -1.487361    -1.707116      26.09
 C       2.513713     0.899990    -2.735847      46.83
 H       2.324823     0.552181    -3.818768      23.95
 C       2.336948     2.715100    -0.935771      37.81
 C       1.608063     3.985189    -0.390983     116.54
 H       1.905361     4.909806    -1.040500      20.68
 O       1.987264     4.367701     0.855327     291.57
 H       2.862251     4.781848     0.792891      29.47
 C       0.064409     3.950824    -0.500417      78.51
 H      -0.416547     3.693175    -1.494228      18.97
 C      -0.577563     5.280077    -0.029011      99.45
 O      -0.170417     6.482353    -0.939491     232.92
 H       0.081837     6.359428    -1.815233      32.50
 H      -0.102969     5.778419     0.778464      23.61
 H      -1.630514     5.258540     0.017791      25.87
 C      -1.002512    -0.763012     0.029286      22.05
 H      -0.336146    -1.607898     0.212912      17.11
 C      -3.059103     0.526066    -0.539274      75.75
 H      -4.164732     0.491201    -0.424842      22.66
 C      -2.396927     1.700266    -0.158717      -2.73
 O      -2.938022     3.013867    -0.427910     167.26
 C      -4.155884     3.125277    -1.264160      79.06
 H      -5.172676     2.422228    -1.044211      22.08
 H      -4.039805     4.232506    -1.391815      23.36
 H      -4.012000     2.676621    -2.532996      22.92
 C      -0.941298     1.776818    -0.069811      10.00
 O      -0.328820     2.982730     0.556459     207.34
 C      -0.260828     0.531932     0.315455       7.17
 H       0.596847     0.510689     0.813605      17.50
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 C      -2.415028    -0.733668    -0.548487      11.11
 C      -3.018918    -2.104320    -1.099815      69.83
 H      -3.636609    -1.666524    -1.908591      19.99
 O      -2.088907    -3.000278    -1.704215     299.51
 H      -2.672019    -3.514806    -2.281265      23.06
 C      -3.970892    -2.846019    -0.002924      80.94
 H      -3.105636    -2.959452     0.845523      16.96
 O      -4.798287    -1.799376     0.553794     348.14
 H      -4.951961    -1.897239     1.723314      22.18
 C      -4.754086    -4.113548    -0.306370      73.44
 O      -4.234645    -4.988590    -1.219635     354.19
 H      -3.366892    -5.228088    -0.810287      30.44
 H      -5.715334    -3.843207    -0.816388      26.92
 H      -5.275876    -4.227279     0.906932      25.27
55
name = lig-etoh-frame_729
 C       2.132757     2.232340    -2.303608      19.79
 H       1.507075     2.816132    -2.927536      17.55
 C       3.138738     1.844402    -0.094897      83.88
 H       3.059435     2.274014     0.857594      17.91
 C       3.513285     0.490049    -0.423221      26.51
 O       4.382113    -0.247437     0.261195     267.23
 C       5.255941     0.458660     1.213710      74.96
 H       4.457246     1.035114     1.670386      25.29
 H       5.943565     1.073469     0.616096      26.04
 H       5.805305    -0.528089     1.678752      23.74
 C       3.335049     0.082489    -1.817186       7.22
 O       3.954138    -0.947681    -2.364854     158.00
 H       4.493606    -1.472199    -1.494248      17.71
 C       2.524209     0.891123    -2.739676      46.50
 H       2.497209     0.448376    -3.711944      24.59
 C       2.330493     2.731792    -0.893151      55.48
 C       1.611317     4.039431    -0.360159     104.67
 H       1.970761     4.845708    -1.222108      19.25
 O       1.992283     4.383338     0.901526     307.71
 H       2.926886     4.663615     0.604204      27.98
 C       0.121649     3.939567    -0.517882      78.71
 H      -0.225367     3.586136    -1.459073      19.49
 C      -0.524630     5.233425    -0.056759      88.35
 O      -0.185247     6.473225    -0.881688     215.21
 H       0.042780     6.294265    -1.933909      25.89
 H      -0.110473     5.548735     0.998602      22.52
 H      -1.674372     5.344089    -0.025295      22.69
 C      -1.060416    -0.744754    -0.015115      33.86
 H      -0.525132    -1.636335     0.519884      17.15
 C      -3.115061     0.548318    -0.527681      53.36
 H      -4.184797     0.501219    -0.661667      19.69
 C      -2.316092     1.714096    -0.202341      -7.48
 O      -2.959787     2.995366    -0.449171     157.54
 C      -4.240540     3.120722    -1.301371     113.39
 H      -5.058795     2.717619    -0.887743      28.30
 H      -4.219335     4.259809    -1.017501      23.85
 H      -4.365159     2.931026    -2.254773      29.12
 C      -0.870701     1.748240    -0.011134      24.75
 O      -0.404549     2.947186     0.483258     223.29
 C      -0.266907     0.510435     0.340061       6.53
 H       0.799662     0.445554     0.923055      15.28
 C      -2.440925    -0.688702    -0.558792      22.80
 C      -3.040909    -2.068616    -1.032194      77.18
 H      -3.737440    -1.864151    -1.911118      18.25
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 O      -2.061850    -3.001957    -1.727884     211.84
 H      -2.834676    -3.540651    -2.340254      18.66
 C      -3.881170    -2.815729    -0.004877     109.31
 H      -3.226244    -3.216223     0.701497      20.85
 O      -4.833144    -1.810592     0.586811     388.15
 H      -4.963603    -1.770586     1.493463      30.47
 C      -4.784765    -4.131050    -0.200102     102.69
 O      -4.245050    -5.029401    -1.219352     338.75
 H      -3.318322    -5.320142    -0.783372      27.39
 H      -5.718399    -3.784846    -0.657363      28.67
 H      -5.090910    -4.399394     0.695177      31.67
55
name = lig-etoh-frame_730
 C       2.157517     2.153273    -2.365358      31.82
 H       1.564785     2.867054    -3.054409      17.64
 C       3.159773     1.857888    -0.036787      87.78
 H       3.127275     2.147200     1.086429      13.47
 C       3.478004     0.571963    -0.504211      18.35
 O       4.344873    -0.205479     0.273910     260.44
 C       5.195923     0.449977     1.178404     111.02
 H       4.584135     1.114923     1.875455      25.64
 H       5.952610     1.195591     0.801482      26.24
 H       5.772869    -0.260947     1.657585      27.67
 C       3.260919     0.070313    -1.810631      14.73
 O       3.986275    -0.977638    -2.273223     200.14
 H       4.816247    -1.202127    -1.841767      22.79
 C       2.566252     0.912247    -2.673528      46.88
 H       2.554820     0.487829    -3.788387      22.56
 C       2.333431     2.678565    -0.921996      75.77
 C       1.638759     4.047559    -0.436839      95.71
 H       1.939152     4.772703    -1.246379      22.62
 O       2.018471     4.414809     0.956962     304.32
 H       3.034135     4.539365     1.072787      29.71
 C       0.138239     3.920817    -0.504629      78.03
 H       0.010617     3.561890    -1.587219      18.81
 C      -0.485456     5.264914    -0.082186     111.64
 O      -0.182232     6.461410    -0.831370     308.02
 H      -0.176918     6.013385    -1.720470      30.25
 H      -0.243290     5.188830     0.954130      25.73
 H      -1.529724     5.076688    -0.076042      25.22
 C      -1.087284    -0.669575    -0.036882      60.20
 H      -0.947312    -1.634607     0.357626      17.83
 C      -3.128246     0.563715    -0.511620      44.12
 H      -4.164936     0.675532    -0.972550      11.93
 C      -2.283311     1.735423    -0.318697       1.28
 O      -2.979068     2.949144    -0.483089     155.73
 C      -4.287612     3.177518    -1.237898      89.72
 H      -5.179534     2.798183    -0.432464      22.05
 H      -4.652279     4.176018    -1.018535      25.50
 H      -4.361038     3.046749    -2.550459      22.63
 C      -0.854620     1.690927     0.098716      19.68
 O      -0.456758     2.926639     0.407999     247.79
 C      -0.319019     0.438256     0.341147      47.35
 H       0.641429     0.381302     0.728300      17.66
 C      -2.393845    -0.693554    -0.536558      33.46
 C      -3.094577    -2.016872    -1.017900      75.76
 H      -3.838411    -1.863031    -1.778240      20.04
 O      -2.056917    -3.000060    -1.748693     274.65
 H      -2.580639    -3.554040    -2.242469      24.82
 C      -3.823110    -2.793442     0.070057      90.46
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 H      -3.100835    -3.345106     0.829573      16.38
 O      -4.860291    -1.823379     0.573419     289.08
 H      -4.783633    -1.861729     1.687297      22.90
 C      -4.825077    -4.074749    -0.179321      64.00
 O      -4.232534    -5.085807    -1.196779     325.67
 H      -3.478812    -5.499642    -0.856162      29.61
 H      -5.786281    -3.684387    -0.559704      27.32
 H      -4.837681    -4.927000     0.880203      24.03
55
name = lig-etoh-frame_731
 C       2.149406     2.163930    -2.331512      31.25
 H       1.759407     2.703421    -3.132502      20.96
 C       3.094923     1.906201    -0.004204      67.59
 H       3.365073     1.970224     1.013816      16.57
 C       3.479292     0.662131    -0.561687      45.00
 O       4.311973    -0.192308     0.273577     223.53
 C       5.140844     0.496737     1.176236     129.59
 H       4.841299     0.979510     2.147966      26.94
 H       5.849780     1.220462     0.757950      30.96
 H       5.800111    -0.263822     1.843090      25.97
 C       3.216434     0.092636    -1.760967      11.66
 O       4.013776    -1.032868    -2.212584     194.27
 H       5.016923    -0.975112    -1.992685      25.18
 C       2.617937     0.889854    -2.683579      51.48
 H       2.519235     0.695510    -3.661255      19.81
 C       2.352040     2.600003    -0.982652      44.54
 C       1.721032     3.990526    -0.494106      85.39
 H       1.975231     4.938535    -1.256276      18.67
 O       2.048281     4.439538     0.987508     313.99
 H       2.932951     4.438070     1.427350      29.66
 C       0.156852     3.889999    -0.530963      78.64
 H       0.015145     3.682966    -1.573438      20.74
 C      -0.488695     5.267306    -0.086914     100.56
 O      -0.172443     6.428312    -0.776462     291.49
 H      -0.236851     6.117513    -1.710043      29.49
 H      -0.262747     5.237329     1.050914      23.00
 H      -1.572400     4.857453    -0.211508      22.49
 C      -1.123082    -0.653420    -0.048181      54.72
 H      -0.907391    -1.800687     0.058134      15.67
 C      -3.083466     0.570344    -0.537913      63.74
 H      -3.960145     0.783536    -1.081008      15.62
 C      -2.320953     1.712033    -0.453451      14.25
 O      -2.992556     2.938400    -0.535060     215.52
 C      -4.352695     3.220191    -1.125371     117.38
 H      -4.966067     2.578806    -0.609113      27.28
 H      -4.734776     4.346357    -1.163229      25.04
 H      -4.246337     2.990335    -2.044235      30.18
 C      -0.955336     1.648122     0.169240       3.68
 O      -0.460897     2.945843     0.363018     225.23
 C      -0.374719     0.382545     0.330740      56.51
 H       0.711781     0.230982     0.669736      15.40
 C      -2.394904    -0.675724    -0.526837      32.60
 C      -3.118025    -2.001362    -1.030270      52.50
 H      -3.972375    -1.631598    -1.725713      19.42
 O      -2.052771    -2.958916    -1.741841     222.79
 H      -2.558262    -3.729394    -2.240970      19.61
 C      -3.818389    -2.818859     0.189012      87.62
 H      -3.039781    -2.996168     0.930150      20.04
 O      -4.865799    -1.843373     0.595399     355.79
 H      -4.554802    -1.956028     1.609469      22.06
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 C      -4.794468    -4.075708    -0.159860      95.20
 O      -4.248875    -5.118083    -1.186720     325.68
 H      -3.536842    -5.660079    -0.665121      26.86
 H      -5.822267    -3.758717    -0.423281      28.18
 H      -4.736662    -4.659598     0.555222      29.32
55
name = lig-etoh-frame_732
 C       2.148991     2.168247    -2.265335      55.96
 H       1.808611     2.760637    -3.164779      24.28
 C       3.014197     1.901494    -0.038282      58.44
 H       3.464426     2.166615     0.960085      20.15
 C       3.531416     0.720160    -0.509775      23.96
 O       4.271165    -0.173276     0.273047     216.32
 C       5.146525     0.534208     1.247913     112.51
 H       4.666947     0.926685     2.196365      24.82
 H       5.724968     1.203199     0.592504      26.62
 H       5.748857    -0.319037     1.556367      25.54
 C       3.250901     0.071761    -1.748759      13.95
 O       4.010403    -1.089806    -2.154625     141.60
 H       5.041182    -0.687281    -2.082327      26.36
 C       2.637332     0.896728    -2.721867      45.37
 H       2.499685     0.661791    -3.903618      17.85
 C       2.354416     2.618672    -1.005521      35.88
 C       1.828281     3.923874    -0.516180      87.43
 H       2.024183     4.899454    -1.025608      18.54
 O       2.040464     4.443282     0.978251     278.79
 H       3.031761     4.316557     1.331014      24.58
 C       0.209254     3.883358    -0.570615      52.16
 H      -0.201981     3.741420    -1.639745      20.36
 C      -0.536766     5.184103    -0.051791      98.54
 O      -0.155580     6.400680    -0.734983     230.26
 H      -0.150898     6.484856    -1.795540      27.33
 H      -0.315312     5.566480     0.920432      23.29
 H      -1.569808     5.021462    -0.286361      24.37
 C      -1.160087    -0.790548    -0.064855      31.92
 H      -0.474010    -1.614270    -0.188078      17.49
 C      -3.034218     0.553280    -0.626618      57.59
 H      -4.046901     0.636014    -1.130052      15.99
 C      -2.365754     1.707041    -0.526898      37.90
 O      -2.985985     2.979308    -0.583894     214.67
 C      -4.380469     3.247355    -0.984278      99.73
 H      -5.117819     2.302706    -0.684803      21.60
 H      -4.471571     4.280982    -1.026060      25.68
 H      -4.217494     2.700894    -2.205668      22.45
 C      -1.106605     1.663338     0.168812      -0.49
 O      -0.439779     2.955893     0.354707     193.90
 C      -0.386366     0.398896     0.338625      22.80
 H       0.689197     0.157120     0.620391      15.85
 C      -2.466588    -0.672513    -0.543795      31.31
 C      -3.125817    -2.013186    -1.037234      60.87
 H      -3.873979    -1.614730    -1.664502      20.82
 O      -2.069804    -2.886270    -1.730532     217.64
 H      -2.621932    -3.791340    -2.006983      17.57
 C      -3.855446    -2.819718     0.226752      79.40
 H      -3.071493    -2.813416     1.051000      17.63
 O      -4.838819    -1.873697     0.655176     358.37
 H      -4.778118    -1.790880     1.652183      26.55
 C      -4.692828    -4.078301    -0.193539      69.79
 O      -4.267387    -5.131494    -1.177785     310.85
 H      -3.733650    -5.651574    -0.468828      25.57
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 H      -5.740794    -3.827064    -0.382405      27.04
 H      -4.832224    -4.690489     1.070159      23.97
55
name = lig-etoh-frame_733
 C       2.151590     2.143269    -2.286403      64.34
 H       1.724617     2.930045    -2.922420      25.83
 C       2.981455     1.864786    -0.060158      75.50
 H       3.251756     2.557885     0.757373      21.10
 C       3.585739     0.684206    -0.446364      21.87
 O       4.240300    -0.140661     0.303439     222.10
 C       5.154428     0.529645     1.304938      98.36
 H       4.473943     0.981973     2.021922      23.81
 H       5.655875     1.298686     0.689120      26.14
 H       5.872252    -0.361808     1.394768      23.15
 C       3.313859     0.070766    -1.790219      13.57
 O       3.997377    -1.112958    -2.094919     220.88
 H       4.834383    -0.846756    -2.105731      30.70
 C       2.638643     0.908728    -2.765161      35.40
 H       2.577322     0.570602    -3.717456      19.48
 C       2.353780     2.701102    -0.977587      36.34
 C       1.854369     3.917983    -0.475104     101.69
 H       2.223708     4.867990    -1.110172      17.73
 O       2.037299     4.405848     0.934262     322.61
 H       2.976503     4.352610     0.947360      28.21
 C       0.235413     3.895777    -0.604676      56.27
 H      -0.213683     3.736014    -1.561031      21.82
 C      -0.568538     5.119610    -0.057941      91.46
 O      -0.122117     6.415866    -0.718030     238.24
 H      -0.096654     6.409832    -1.666703      31.91
 H      -0.410670     5.581168     0.976673      22.76
 H      -1.684311     5.093651    -0.213055      23.75
 C      -1.128570    -0.887996    -0.073751      25.92
 H      -0.275876    -1.556217    -0.371484      17.87
 C      -3.077404     0.519857    -0.781427      43.86
 H      -4.112373     0.386255    -1.042756      19.84
 C      -2.403011     1.770540    -0.525116      17.20
 O      -2.965008     3.034962    -0.615893     227.49
 C      -4.354215     3.133778    -0.943931     124.19
 H      -5.226201     2.674009    -0.478002      26.83
 H      -4.417883     4.301780    -0.754739      24.84
 H      -4.508787     2.985757    -1.907355      29.28
 C      -1.172602     1.706181     0.124205       1.55
 O      -0.415662     2.926030     0.378968     188.27
 C      -0.466623     0.420335     0.319072       7.89
 H       0.579180     0.372949     0.608537      17.06
 C      -2.500455    -0.769190    -0.562622      30.02
 C      -3.121566    -2.032779    -1.013693      69.25
 H      -3.934305    -1.819581    -1.849121      20.04
 O      -2.118734    -2.812597    -1.708962     298.61
 H      -2.557758    -3.576549    -1.743223      25.21
 C      -3.876215    -2.774613     0.204620      92.55
 H      -3.121299    -3.054649     1.029368      19.20
 O      -4.820577    -1.894400     0.714720     335.61
 H      -5.113635    -1.700313     1.759437      24.86
 C      -4.605484    -4.132345    -0.134312     113.91
 O      -4.277307    -5.126567    -1.133994     386.62
 H      -3.775563    -5.719035    -0.604229      32.76
 H      -5.591549    -3.745610    -0.489404      29.15
 H      -4.870628    -4.393131     0.731612      32.12
55
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name = lig-etoh-frame_736
 C       2.145665     2.199340    -2.369040      22.66
 H       1.481257     2.521456    -3.086176      19.70
 C       3.081371     1.825744    -0.048764      67.63
 H       3.031852     1.740973     0.992785      16.47
 C       3.526722     0.635802    -0.453870       9.41
 O       4.331648    -0.234698     0.522683     214.22
 C       5.139297     0.525314     1.469635      86.95
 H       4.611979     0.710910     2.457337      25.44
 H       5.608421     1.362249     0.973470      27.29
 H       5.931749    -0.326894     1.780071      24.35
 C       3.571907     0.190266    -1.816901      16.15
 O       3.845627    -1.175936    -2.030544     246.17
 H       4.679251    -1.476694    -1.749541      24.85
 C       2.688148     0.951096    -2.705498      61.46
 H       2.456632     0.576386    -3.738718      25.24
 C       2.292942     2.650596    -1.027985      59.63
 C       1.613811     4.076359    -0.562598     101.33
 H       1.659377     5.129143    -1.133200      18.52
 O       2.152184     4.244552     0.810603     305.71
 H       2.731751     4.969452     0.954386      34.48
 C       0.111570     3.914629    -0.559405      77.40
 H      -0.130135     3.500178    -1.562074      18.51
 C      -0.579053     5.182512    -0.108343      99.99
 O      -0.045035     6.385493    -0.685082     248.00
 H       0.149418     6.288754    -1.629248      32.35
 H      -0.400444     5.277370     1.004762      23.73
 H      -1.674860     5.180098    -0.429553      23.50
 C      -1.150070    -0.762216    -0.207790      43.94
 H      -0.682075    -1.617226     0.369201      16.31
 C      -3.077594     0.454587    -0.975368      56.44
 H      -4.077119     0.472583    -1.394693      20.79
 C      -2.528743     1.689276    -0.504945       6.17
 O      -2.952483     3.081261    -0.748977     182.05
 C      -4.455306     3.218211    -0.702851      87.96
 H      -4.595290     2.169929    -0.125408      20.70
 H      -4.724454     4.219305    -0.499817      24.37
 H      -4.855176     2.623562    -1.845319      21.99
 C      -1.189962     1.734891    -0.110862      22.74
 O      -0.306079     2.758293     0.469121     136.01
 C      -0.637336     0.497863     0.186308      16.72
 H       0.438993     0.314353     0.734397      14.14
 C      -2.438910    -0.716665    -0.698937      19.76
 C      -3.293249    -2.066194    -1.008656      70.80
 H      -4.097215    -1.680282    -1.538570      21.17
 O      -2.180747    -2.817465    -1.663316     261.60
 H      -2.295377    -3.749442    -1.719979      20.34
 C      -3.754516    -2.839441     0.204860      97.69
 H      -2.927038    -2.842279     0.901523      17.96
 O      -4.841899    -1.920262     0.786643     305.07
 H      -4.791294    -1.945159     1.878694      23.77
 C      -4.697329    -4.039603    -0.128023      76.91
 O      -4.196423    -5.143135    -1.035567     318.08
 H      -3.387471    -5.389010    -0.472651      25.76
 H      -5.692577    -3.721351    -0.500134      26.23
 H      -5.011290    -4.692352     1.026537      24.29
55
name = lig-etoh-frame_737
 C       2.161560     2.151534    -2.357888       0.80
 H       1.440410     2.697768    -3.094583      16.06
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 C       3.062119     1.832946    -0.065391      68.10
 H       2.908581     2.029828     1.063837      13.81
 C       3.629088     0.593329    -0.391942      15.54
 O       4.321537    -0.266902     0.530678     225.04
 C       5.156186     0.498944     1.602607      82.42
 H       4.521314     0.865321     2.401378      26.90
 H       5.562998     1.347171     1.027129      28.62
 H       5.934499    -0.256065     1.645708      26.21
 C       3.607282     0.174363    -1.823313      16.82
 O       3.773182    -1.191582    -2.066196     152.40
 H       4.693262    -1.369267    -1.414129      19.35
 C       2.752147     0.950913    -2.686801      46.06
 H       2.498195     0.511090    -3.712312      24.71
 C       2.243400     2.714939    -1.026232      66.58
 C       1.617256     4.015740    -0.611505     107.69
 H       1.620925     5.001811    -1.104488      19.06
 O       2.158434     4.207467     0.804503     267.67
 H       2.765773     5.032294     0.745689      31.67
 C       0.057795     3.837673    -0.520574      74.47
 H      -0.521406     3.640669    -1.466979      17.86
 C      -0.618242     5.197232    -0.112069     101.55
 O      -0.009091     6.369277    -0.681624     195.89
 H       0.102338     6.434154    -1.739793      29.47
 H      -0.551692     5.646510     0.894889      23.55
 H      -1.665869     5.284707    -0.277288      25.64
 C      -1.231147    -0.699899    -0.214128      39.07
 H      -0.822695    -1.418732     0.442897      18.19
 C      -3.063150     0.543363    -0.953033      51.87
 H      -3.958794     0.401864    -1.617460      18.06
 C      -2.515821     1.721789    -0.583447      23.47
 O      -2.984894     3.057185    -0.809595     233.95
 C      -4.458093     3.157267    -0.631521     130.40
 H      -5.156209     2.496437     0.031664      25.58
 H      -4.823169     4.203965    -0.435116      25.58
 H      -4.854872     2.899138    -1.476243      28.99
 C      -1.177067     1.727922    -0.127009      29.52
 O      -0.292804     2.737481     0.436726     191.20
 C      -0.521341     0.470606     0.157432      19.50
 H       0.299472     0.361445     0.712937      16.10
 C      -2.516628    -0.717726    -0.789596      41.49
 C      -3.247396    -2.025301    -1.015977      58.23
 H      -4.159966    -1.729416    -1.710526      19.98
 O      -2.177261    -2.870302    -1.685521     170.55
 H      -2.689683    -3.895262    -1.762424      12.64
 C      -3.809731    -2.840310     0.223357      79.07
 H      -2.925420    -3.045265     1.055776      15.03
 O      -4.803921    -1.955408     0.821735     354.45
 H      -4.831349    -1.773130     1.778132      26.84
 C      -4.752414    -4.062122    -0.115590      98.49
 O      -4.146502    -5.121178    -1.013002     348.20
 H      -3.420806    -5.374195    -0.285977      25.49
 H      -5.729840    -3.669892    -0.397294      29.06
 H      -4.951667    -4.355986     0.769879      31.21
55
name = lig-etoh-frame_738
 C       2.150303     2.153037    -2.311076      71.55
 H       1.611955     2.722003    -3.005661      25.88
 C       2.986671     1.881595    -0.073743      44.32
 H       2.959809     2.436784     0.844287      17.45
 C       3.750342     0.557647    -0.377002      41.87
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 O       4.301904    -0.273419     0.539038     229.68
 C       5.144342     0.461744     1.659929      78.50
 H       4.507291     0.888794     2.477096      23.54
 H       5.540069     1.378678     1.205769      27.98
 H       6.120273    -0.256999     1.900873      22.73
 C       3.569920     0.163898    -1.781611      39.41
 O       3.744417    -1.193323    -2.090861     161.36
 H       4.356513    -1.491113    -1.454408      23.36
 C       2.840820     0.908155    -2.687777      40.38
 H       2.638218     0.466003    -3.619525      19.10
 C       2.266814     2.700086    -1.043959      10.67
 C       1.600229     3.926035    -0.586790      99.31
 H       1.961148     4.820390    -1.370177      13.97
 O       2.130835     4.191958     0.775077     291.27
 H       2.845741     4.868074     0.617490      28.89
 C      -0.027567     3.782583    -0.464755      77.90
 H      -0.533855     3.659975    -1.396976      19.49
 C      -0.657976     5.247112    -0.085249      89.18
 O       0.046293     6.389125    -0.714369     231.32
 H      -0.106488     6.203134    -1.648608      30.24
 H      -0.618041     5.556739     1.011791      24.15
 H      -1.814167     5.145924    -0.282692      23.60
 C      -1.283768    -0.643474    -0.166106      36.65
 H      -0.959934    -1.695661     0.232979      15.98
 C      -3.123398     0.593261    -0.993457      45.56
 H      -3.962293     0.654731    -1.659777      16.07
 C      -2.438859     1.835312    -0.661526      13.16
 O      -3.055112     3.017634    -0.846570     218.61
 C      -4.480268     3.110157    -0.560562      97.74
 H      -5.186848     2.736841     0.375296      23.77
 H      -4.638162     4.211616    -0.338537      25.11
 H      -5.092196     3.115899    -1.739826      22.00
 C      -1.083496     1.690511    -0.083004      10.69
 O      -0.309295     2.738892     0.382044     226.25
 C      -0.485884     0.450418     0.081958      44.99
 H       0.486522     0.512895     0.791419      13.52
 C      -2.557007    -0.726568    -0.833741      27.27
 C      -3.184371    -1.999508    -1.050038      81.56
 H      -3.955022    -2.031561    -1.773115      22.30
 O      -2.213200    -2.954572    -1.710051     267.83
 H      -2.822518    -3.598513    -1.815164      22.85
 C      -3.879930    -2.808824     0.255604      83.17
 H      -3.132877    -3.275474     0.889388      18.79
 O      -4.784080    -1.970840     0.818790     305.12
 H      -4.579220    -1.881975     1.994812      19.46
 C      -4.772814    -4.067115    -0.137750      60.77
 O      -4.106528    -5.071447    -0.959464     356.39
 H      -3.452904    -5.632263    -0.498381      28.03
 H      -5.694101    -3.637442    -0.628224      27.94
 H      -5.005688    -4.458773     1.126571      26.25
55
name = lig-etoh-frame_739
 C       2.170715     2.122194    -2.301288      65.43
 H       1.669379     2.691017    -3.108982      24.22
 C       2.955427     1.892620    -0.091398      62.29
 H       3.192213     2.549532     0.788927      18.34
 C       3.788325     0.637494    -0.400280      20.00
 O       4.308555    -0.270826     0.580801     249.62
 C       5.134449     0.422023     1.678804     108.01
 H       4.519824     0.610267     2.567482      25.81
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 H       5.553564     1.363708     1.319214      26.06
 H       5.880949    -0.153499     2.151737      25.83
 C       3.516514     0.123002    -1.681358      13.88
 O       3.722263    -1.189865    -2.123424     199.95
 H       4.247428    -1.761471    -1.467707      24.21
 C       2.890054     0.923452    -2.677628      34.21
 H       2.777166     0.381177    -3.737786      19.21
 C       2.329146     2.595572    -1.043614      28.52
 C       1.578901     3.862717    -0.557174     118.23
 H       1.982936     4.495264    -1.330767      19.56
 O       2.081823     4.202606     0.730612     315.87
 H       2.944700     4.607138     0.678260      32.16
 C      -0.075317     3.822202    -0.444985      69.02
 H      -0.332635     3.515034    -1.536310      18.84
 C      -0.699854     5.291440    -0.014643     100.97
 O       0.075400     6.389361    -0.754717     218.97
 H      -0.115267     6.040848    -1.692793      28.38
 H      -0.586344     5.262678     1.060604      25.64
 H      -1.665598     5.148005    -0.401901      24.90
 C      -1.326526    -0.691949    -0.109254      45.53
 H      -1.008895    -1.696330    -0.148311      18.39
 C      -3.167951     0.632621    -1.069067      20.93
 H      -4.131059     0.971317    -1.577538      17.23
 C      -2.330435     1.858211    -0.720081      -4.28
 O      -3.137388     2.997792    -0.864332     217.01
 C      -4.555235     3.133285    -0.552409     107.44
 H      -4.637182     2.638294     0.477983      25.43
 H      -4.377685     4.222256    -0.284903      24.68
 H      -5.134437     3.068530    -1.310479      27.63
 C      -1.031394     1.683831    -0.064682       9.20
 O      -0.337850     2.743328     0.363238     229.92
 C      -0.464745     0.434533     0.041892      53.32
 H       0.475960     0.470226     0.529024      17.06
 C      -2.551901    -0.636021    -0.825484      21.51
 C      -3.143124    -2.057546    -1.088860      74.22
 H      -3.983566    -2.045073    -1.876414      21.25
 O      -2.242256    -3.019533    -1.725170     210.19
 H      -2.961489    -3.784877    -1.970661      16.93
 C      -3.927962    -2.795100     0.225763      70.97
 H      -3.063697    -3.412504     0.835871      18.50
 O      -4.779238    -1.944029     0.867994     342.09
 H      -4.591508    -2.121561     1.804503      25.65
 C      -4.773909    -4.070711    -0.107331     108.34
 O      -4.092305    -5.013467    -0.923942     357.45
 H      -3.447161    -5.731849    -0.574322      27.29
 H      -5.575590    -3.844839    -0.822749      28.40
 H      -5.109442    -4.488236     0.686415      31.48
55
name = lig-etoh-frame_740
 C       2.225558     2.044891    -2.378041      55.14
 H       1.658668     2.618059    -3.162974      22.35
 C       3.042917     1.838892    -0.060210      67.46
 H       3.385107     2.305178     0.869467      18.44
 C       3.762354     0.745624    -0.400180      34.11
 O       4.338636    -0.244766     0.633078     254.58
 C       5.083680     0.391615     1.686947      95.69
 H       4.341878     0.444854     2.550351      23.73
 H       5.575736     1.347805     1.410376      24.91
 H       5.873799    -0.416571     2.233319      22.88
 C       3.464517     0.065907    -1.598975       9.51
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 O       3.711057    -1.184330    -2.150908     170.32
 H       4.147298    -1.954935    -1.476710      22.49
 C       2.906293     0.941388    -2.673404      42.79
 H       2.908072     0.542163    -3.596194      21.36
 C       2.319976     2.511300    -1.018737      27.17
 C       1.561192     3.800520    -0.530198     104.56
 H       1.817437     4.646516    -1.436619      16.34
 O       2.023727     4.238482     0.704285     282.60
 H       3.059993     4.311068     0.772722      26.12
 C      -0.039863     3.902142    -0.508402      66.04
 H      -0.239128     3.575224    -1.481660      19.11
 C      -0.682539     5.288581     0.015377      88.80
 O       0.066293     6.356893    -0.774537     203.67
 H       0.141001     6.073067    -1.791909      26.57
 H      -0.535959     5.241793     1.157315      22.95
 H      -1.756684     5.368785    -0.423048      22.09
 C      -1.344177    -0.749237    -0.102219      34.61
 H      -0.805363    -1.746203    -0.290201      17.29
 C      -3.140427     0.705348    -1.139918      42.30
 H      -4.159951     0.925972    -1.393465      19.80
 C      -2.312487     1.782793    -0.773627       3.87
 O      -3.161054     2.998651    -0.895573     169.01
 C      -4.539687     3.186796    -0.468704      69.39
 H      -4.507117     2.445873     0.431801      22.85
 H      -4.510868     4.312394    -0.223418      23.00
 H      -5.598864     2.806123    -1.318466      21.47
 C      -1.059442     1.705178    -0.105285      12.18
 O      -0.362257     2.762220     0.403118     190.04
 C      -0.478087     0.385256     0.027462      22.48
 H       0.641504     0.259319     0.331997      15.47
 C      -2.567924    -0.554091    -0.799427      14.16
 C      -3.181358    -2.135591    -1.135211      72.65
 H      -3.976367    -1.771496    -1.792943      22.27
 O      -2.269867    -3.084712    -1.738938     235.51
 H      -2.765722    -3.968888    -2.023041      18.66
 C      -3.915424    -2.831002     0.153287      91.37
 H      -3.061453    -3.112519     0.808379      21.03
 O      -4.781619    -1.884505     0.907664     265.24
 H      -4.832533    -2.268100     2.026473      22.34
 C      -4.763685    -4.047671    -0.145027      89.82
 O      -4.073268    -4.985726    -0.939044     324.10
 H      -3.424823    -5.442205    -0.302716      26.52
 H      -5.621641    -3.876707    -0.851285      25.91
 H      -5.465106    -4.687943     0.805757      25.83
55
name = lig-etoh-frame_741
 C       2.259691     2.031539    -2.417722      33.35
 H       1.695827     2.521403    -3.129979      19.13
 C       3.156229     1.832162     0.000961      54.68
 H       3.337213     2.092103     1.043411      17.28
 C       3.763054     0.689332    -0.375834      39.15
 O       4.368988    -0.191391     0.645115     260.37
 C       5.024701     0.326388     1.745027     126.74
 H       4.266005     0.576026     2.486518      25.90
 H       5.569501     1.255411     1.562015      28.33
 H       5.728005    -0.421077     1.919882      25.43
 C       3.413622     0.045243    -1.594385      34.33
 O       3.710191    -1.197937    -2.155743     254.77
 H       4.035808    -1.735992    -1.538010      32.21
 C       2.948958     0.873124    -2.639504      42.41
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 H       3.034897     0.542893    -3.797069      19.61
 C       2.242496     2.473817    -0.997341      31.16
 C       1.555088     3.792201    -0.561639     113.55
 H       1.693117     4.624164    -1.298003      17.85
 O       1.982474     4.288879     0.709525     302.57
 H       2.928212     4.047573     0.792399      26.77
 C       0.038958     3.949897    -0.554999      55.50
 H      -0.438287     3.739486    -1.605204      15.68
 C      -0.628288     5.260496    -0.035919     104.37
 O       0.052146     6.324766    -0.768378     269.77
 H       0.225462     6.075892    -1.680795      31.34
 H      -0.461561     5.527058     0.992304      24.19
 H      -1.678808     5.457244    -0.104678      24.42
 C      -1.314560    -0.775120    -0.161731      34.66
 H      -0.772360    -1.700076    -0.156123      17.64
 C      -3.073036     0.708137    -1.184344      52.74
 H      -4.161372     0.724738    -1.371070      23.65
 C      -2.388522     1.754527    -0.808901      14.70
 O      -3.129893     3.023463    -0.948906     214.38
 C      -4.529872     3.194665    -0.394057     117.06
 H      -4.758180     2.422424     0.470913      24.29
 H      -4.835605     4.219096    -0.154489      25.94
 H      -5.259228     2.840688    -0.861634      29.54
 C      -1.087931     1.700588    -0.161524      10.38
 O      -0.397228     2.798015     0.454333     140.74
 C      -0.511489     0.343137     0.037382      26.56
 H       0.590468     0.108523     0.089345      16.89
 C      -2.595765    -0.586631    -0.766887      17.78
 C      -3.284814    -2.160222    -1.163792      60.35
 H      -4.034769    -1.747520    -1.873928      20.35
 O      -2.279275    -3.135067    -1.758054     244.44
 H      -2.712514    -3.925547    -1.878576      23.04
 C      -3.900846    -2.836299     0.110380      91.29
 H      -2.978625    -2.835271     0.856841      16.87
 O      -4.786053    -1.838117     0.939236     355.45
 H      -4.866277    -2.028568     1.789664      31.11
 C      -4.830554    -4.050437    -0.191414     101.98
 O      -4.035741    -4.992074    -0.959838     382.56
 H      -3.367840    -5.198925    -0.272950      30.15
 H      -5.671169    -3.592617    -0.734516      27.93
 H      -5.218229    -4.387473     0.621647      30.68
55
name = lig-etoh-frame_742
 C       2.286026     2.054387    -2.351280      75.94
 H       1.681061     2.560348    -3.229872      17.65
 C       3.205947     1.889671     0.023091      88.84
 H       3.092835     2.049173     1.150591      14.75
 C       3.779159     0.518634    -0.328487       6.73
 O       4.377776    -0.149589     0.585651     242.29
 C       4.962819     0.301209     1.819512      92.36
 H       4.297169     0.624671     2.670253      25.47
 H       5.610922     1.214225     1.653933      26.07
 H       5.778133    -0.629394     1.925991      22.23
 C       3.397164     0.032513    -1.641674      16.35
 O       3.710471    -1.212512    -2.148336     215.76
 H       4.158289    -1.739714    -1.338602      23.42
 C       2.980408     0.789024    -2.661735      42.00
 H       3.125703     0.466673    -3.612486      22.83
 C       2.187786     2.456394    -0.968753      69.69
 C       1.544590     3.818698    -0.601837     103.70
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 H       1.969331     4.671429    -1.403279      21.07
 O       1.948936     4.330045     0.726934     314.83
 H       2.828702     3.998633     0.853489      28.09
 C       0.053279     3.929018    -0.574593      77.61
 H      -0.475027     3.836462    -1.471602      19.05
 C      -0.531705     5.256194    -0.092868      99.14
 O       0.042354     6.323656    -0.742334     234.12
 H       0.133895     6.022054    -1.796600      27.19
 H      -0.201580     5.657271     0.940423      21.79
 H      -1.696025     5.198538    -0.011148      22.98
 C      -1.292139    -0.780442    -0.259506      43.92
 H      -0.894931    -1.795412     0.030131      16.57
 C      -3.056141     0.558525    -1.212385      34.81
 H      -4.117156     0.606247    -1.569460      23.22
 C      -2.450397     1.850649    -0.791892      -9.73
 O      -3.094894     3.066454    -0.996163     196.86
 C      -4.470653     3.160200    -0.280220      74.99
 H      -4.705289     2.615763     0.709760      23.16
 H      -4.932391     4.231859    -0.030841      23.40
 H      -5.348455     2.660292    -1.225323      21.31
 C      -1.094844     1.677292    -0.195614      -2.87
 O      -0.455242     2.827655     0.467473     139.48
 C      -0.556519     0.357171     0.028877      42.00
 H       0.510572     0.212365     0.110332      17.26
 C      -2.610197    -0.725725    -0.752747      17.02
 C      -3.385188    -2.116135    -1.178022      52.58
 H      -4.108348    -2.058425    -2.048803      18.78
 O      -2.284738    -3.132618    -1.772081     135.90
 H      -2.940100    -4.063787    -1.670034      11.10
 C      -3.901255    -2.774663     0.129044      91.33
 H      -3.053721    -3.011790     0.724129      18.59
 O      -4.789840    -1.789052     0.878261     266.01
 H      -4.688368    -1.999120     2.062747      20.75
 C      -4.862731    -3.996139    -0.268855      59.47
 O      -4.025364    -5.001799    -0.986007     299.19
 H      -3.184698    -5.307690    -0.399356      22.31
 H      -5.686972    -3.435127    -0.764485      26.03
 H      -5.114163    -4.393925     0.966646      25.59
55
name = lig-etoh-frame_743
 C       2.309775     2.045521    -2.277097      78.91
 H       1.842896     2.561812    -3.025263      20.43
 C       3.190811     1.883648    -0.012115      97.41
 H       2.943234     2.120572     0.990262      14.09
 C       3.689328     0.494689    -0.321192      14.99
 O       4.415049    -0.183547     0.551149     240.49
 C       4.957559     0.280036     1.885063     114.47
 H       4.297127     0.405867     2.746708      28.06
 H       5.571235     1.130060     1.682615      27.84
 H       5.492739    -0.496519     2.244402      27.67
 C       3.445943    -0.016319    -1.655031      11.56
 O       3.725821    -1.268297    -2.106524     164.08
 H       4.366515    -1.745001    -1.367954      20.19
 C       2.942161     0.828505    -2.680500      35.02
 H       3.132343     0.292129    -3.729784      20.82
 C       2.206776     2.455004    -0.927666      78.20
 C       1.575376     3.874519    -0.636817      99.53
 H       2.089515     4.512352    -1.409468      23.07
 O       1.912333     4.357099     0.735097     311.35
 H       2.888299     4.106615     0.975448      28.19
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 C       0.020225     3.872800    -0.546642      79.87
 H      -0.443830     3.630816    -1.583324      18.98
 C      -0.442386     5.258747    -0.056357     115.64
 O       0.039444     6.357232    -0.780074     304.75
 H       0.007215     6.200424    -1.705886      33.60
 H      -0.073864     5.296107     0.938307      26.79
 H      -1.471603     4.960601    -0.178141      24.29
 C      -1.284136    -0.824211    -0.341426      49.77
 H      -0.987808    -1.770389     0.136557      16.86
 C      -3.069914     0.422446    -1.209199      21.16
 H      -3.968059     0.517625    -1.814624      22.87
 C      -2.473299     1.873813    -0.762638     -25.36
 O      -3.083773     3.117378    -1.009432     197.48
 C      -4.468979     3.100324    -0.243449      98.25
 H      -4.275938     2.716188     0.883090      22.71
 H      -4.597601     4.153726    -0.130814      26.25
 H      -4.943514     2.760600    -0.936077      28.14
 C      -1.134644     1.696837    -0.206443       4.99
 O      -0.518292     2.845644     0.431259     191.60
 C      -0.602165     0.407895    -0.009463      28.37
 H       0.524912     0.454202     0.429522      14.20
 C      -2.632156    -0.871909    -0.806864      20.76
 C      -3.413061    -2.058712    -1.185556      74.82
 H      -4.125366    -2.184183    -1.974819      19.62
 O      -2.331237    -3.121650    -1.765780     180.03
 H      -2.848801    -3.859581    -1.629055      17.85
 C      -3.957143    -2.688222     0.139713      78.01
 H      -3.067851    -3.360614     0.647812      15.38
 O      -4.777630    -1.762365     0.836706     373.26
 H      -4.498200    -1.894149     1.675334      29.08
 C      -4.830184    -3.926172    -0.242049      99.82
 O      -4.037735    -5.005236    -1.022053     353.98
 H      -3.389420    -5.480482    -0.504919      30.18
 H      -5.699298    -3.706689    -0.909639      27.24
 H      -5.139984    -4.367745     0.548226      30.41
55
name = lig-etoh-frame_744
 C       2.326935     2.011785    -2.226292      60.09
 H       1.856791     2.761382    -2.987065      18.97
 C       3.113084     1.811942    -0.071345      68.16
 H       3.052201     2.218574     1.009832      14.06
 C       3.552965     0.576438    -0.346402      31.31
 O       4.483340    -0.272667     0.566246     209.05
 C       4.935955     0.262246     1.917588      89.65
 H       4.022919     0.374044     2.603756      25.76
 H       5.568058     1.197185     1.777179      25.83
 H       5.506051    -0.668059     2.527883      24.21
 C       3.505368    -0.036969    -1.656457      21.44
 O       3.765881    -1.354873    -2.042596     190.37
 H       4.457142    -1.701803    -1.612119      24.68
 C       2.902209     0.867788    -2.674107      44.86
 H       2.881283     0.478724    -3.672420      22.17
 C       2.287377     2.479889    -0.892080      71.89
 C       1.622845     3.875579    -0.610129      91.77
 H       2.047226     4.576265    -1.552719      20.19
 O       1.891360     4.371365     0.734646     288.84
 H       2.845272     4.413543     0.967802      30.37
 C       0.007072     3.804033    -0.559345      88.25
 H      -0.277445     3.463492    -1.529465      20.99
 C      -0.379157     5.209266    -0.016545      92.25
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 O       0.037460     6.422531    -0.804556     224.68
 H      -0.037032     6.229252    -1.861940      26.63
 H      -0.074570     5.056905     1.076552      23.33
 H      -1.515255     5.164662    -0.174913      22.73
 C      -1.273843    -0.865872    -0.366961      32.77
 H      -0.813605    -1.736998     0.095560      18.15
 C      -3.097020     0.385879    -1.188671      40.69
 H      -3.874459     0.429206    -2.023997      21.08
 C      -2.474733     1.778611    -0.761256      -6.92
 O      -3.077527     3.132112    -0.994029     180.83
 C      -4.368314     3.092175    -0.176167      64.28
 H      -4.097744     2.597106     0.696408      25.08
 H      -4.400100     4.291663    -0.266126      22.29
 H      -5.292062     2.381099    -0.993159      21.59
 C      -1.222879     1.758580    -0.206398       8.22
 O      -0.570132     2.857438     0.369633     231.21
 C      -0.629683     0.439513    -0.043073      26.55
 H       0.171933     0.508925     0.592578      17.28
 C      -2.620262    -0.902976    -0.914924      18.58
 C      -3.369975    -2.082824    -1.179907      81.92
 H      -4.257738    -1.889074    -1.912613      22.41
 O      -2.384066    -3.066569    -1.748581     183.92
 H      -2.890095    -4.062622    -1.659877      11.86
 C      -4.011292    -2.672606     0.104052      95.57
 H      -3.244713    -3.101547     0.655097      21.86
 O      -4.757384    -1.735178     0.781006     337.48
 H      -4.436492    -1.763552     1.860647      23.28
 C      -4.785392    -3.880872    -0.262086      98.32
 O      -4.075237    -4.989934    -1.067762     243.70
 H      -3.590400    -5.618367    -0.373371      25.35
 H      -5.600087    -3.937725    -0.997049      24.53
 H      -5.416321    -4.557776     0.677729      25.06
55
name = lig-etoh-frame_745
 C       2.297865     2.048729    -2.214321      52.77
 H       1.912307     2.752975    -2.924255      21.40
 C       3.012436     1.766783    -0.011803      57.45
 H       3.382422     2.151840     0.900244      21.79
 C       3.523144     0.538486    -0.365444      34.79
 O       4.536851    -0.344743     0.585622     159.08
 C       4.885503     0.212256     1.943173     121.14
 H       3.910537     0.527642     2.302247      25.12
 H       5.467988     1.110253     1.964526      27.50
 H       5.434890    -0.500567     2.351838      27.93
 C       3.526210    -0.014799    -1.678012      46.01
 O       3.789951    -1.417283    -1.980287     111.14
 H       4.884441    -1.710831    -1.723828      16.80
 C       2.889634     0.833903    -2.622043      45.36
 H       2.643761     0.680163    -3.744615      21.04
 C       2.355968     2.554271    -0.920192      45.29
 C       1.667520     3.833818    -0.560566     121.11
 H       1.831946     4.618704    -1.380946      19.28
 O       1.892400     4.384839     0.731056     301.48
 H       2.805511     4.721527     0.832149      28.35
 C       0.052685     3.759235    -0.603390      65.05
 H      -0.265450     3.498931    -1.652095      18.78
 C      -0.394022     5.150278    -0.023586      87.71
 O       0.038829     6.477031    -0.808795     223.96
 H       0.071108     6.096987    -1.718294      29.44
 H      -0.100146     5.276826     0.996246      23.91
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 H      -1.428732     5.460396     0.074087      23.41
 C      -1.255030    -0.847541    -0.351038      28.94
 H      -0.582257    -1.728244    -0.088787      18.50
 C      -3.130458     0.439868    -1.194121      62.14
 H      -3.872559     0.448847    -1.936108      19.38
 C      -2.518332     1.656497    -0.815447       6.64
 O      -3.072694     3.070762    -0.967538     225.82
 C      -4.276140     3.104738    -0.223057     121.26
 H      -4.115911     2.395263     0.799195      24.20
 H      -4.627239     4.076073    -0.079466      28.05
 H      -5.102439     2.585163    -0.385599      29.37
 C      -1.291487     1.769203    -0.195862      11.06
 O      -0.613822     2.861186     0.315481     218.04
 C      -0.698985     0.438662    -0.078830      18.04
 H       0.118339     0.382896     0.841875      17.15
 C      -2.525897    -0.829052    -1.002809       8.83
 C      -3.335944    -2.157330    -1.210079      92.94
 H      -4.104765    -1.650823    -1.777715      24.50
 O      -2.454333    -3.025961    -1.732431     276.87
 H      -2.792807    -3.966303    -1.748003      18.22
 C      -4.029225    -2.689891     0.052869      80.73
 H      -3.113886    -2.785145     0.878289      19.06
 O      -4.747349    -1.685179     0.757856     343.51
 H      -4.727357    -1.692051     1.817072      27.23
 C      -4.832106    -3.959493    -0.289931     102.34
 O      -4.101561    -4.978534    -1.089440     311.40
 H      -3.718679    -5.561393    -0.387155      27.67
 H      -5.626884    -3.618201    -1.026979      27.37
 H      -5.240939    -4.253175     0.547886      30.11
55
name = lig-etoh-frame_746
 C       2.273262     2.105671    -2.221894      68.08
 H       1.849522     2.696112    -3.066984      23.46
 C       2.955421     1.715740     0.103707      88.39
 H       3.573495     2.150467     0.955460      25.24
 C       3.594890     0.415058    -0.346957     -17.99
 O       4.561465    -0.379206     0.578692     147.64
 C       4.787423     0.190161     1.906107      90.18
 H       3.808171     0.544099     2.360747      24.37
 H       5.479877     1.108377     1.955502      24.76
 H       5.430506    -0.713411     2.464373      23.26
 C       3.520004    -0.026570    -1.706095      19.08
 O       3.846326    -1.447257    -1.908598     229.55
 H       4.789213    -1.488571    -1.991728      25.50
 C       2.860626     0.798043    -2.588114      33.77
 H       2.594132     0.648557    -3.665414      21.30
 C       2.407782     2.629795    -0.957108      38.07
 C       1.671013     3.797742    -0.511013     119.92
 H       1.673775     4.770665    -1.244554      15.88
 O       1.925806     4.391422     0.744616     275.23
 H       2.761240     4.997255     0.638441      26.42
 C       0.096473     3.753156    -0.652998      58.87
 H      -0.270002     3.690915    -1.699243      18.31
 C      -0.437074     5.168564    -0.057374      75.60
 O       0.045634     6.487600    -0.784203     210.94
 H       0.196006     6.166450    -1.743549      28.02
 H       0.093080     5.451580     0.895352      20.96
 H      -1.530085     5.327059     0.139478      23.47
 C      -1.229195    -0.788426    -0.348952      56.68
 H      -0.633292    -1.653755    -0.312648      20.51
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 C      -3.155639     0.488981    -1.228110      49.68
 H      -4.175618     0.558748    -1.778282      17.53
 C      -2.572821     1.631310    -0.882456      13.29
 O      -3.073787     2.955434    -0.964581     265.84
 C      -4.187264     3.098753    -0.195260     117.82
 H      -4.052467     2.720103     0.788589      27.70
 H      -4.746696     4.074077     0.221578      24.75
 H      -5.334138     2.447647    -0.384384      24.31
 C      -1.316490     1.682263    -0.191804      10.55
 O      -0.657232     2.851183     0.273551     195.37
 C      -0.731412     0.439701    -0.025789      50.05
 H       0.039732     0.335727     0.588358      21.07
 C      -2.420341    -0.760457    -1.044389      12.63
 C      -3.325365    -2.121228    -1.218105      77.15
 H      -4.137634    -1.756082    -1.982114      22.16
 O      -2.475796    -3.028157    -1.760584     276.39
 H      -2.888873    -3.899758    -1.753610      20.97
 C      -3.963968    -2.699772     0.074880      93.33
 H      -3.192464    -2.880371     0.690464      26.15
 O      -4.781127    -1.615946     0.719116     333.30
 H      -4.844556    -1.885741     1.670815      27.65
 C      -4.892301    -3.998782    -0.371754      73.01
 O      -4.138529    -4.972933    -1.092107     319.17
 H      -3.626886    -5.532801    -0.485892      28.13
 H      -5.632060    -3.353245    -0.869287      27.32
 H      -5.315703    -4.319780     0.824971      26.36
55
name = lig-etoh-frame_747
 C       2.285783     2.127110    -2.259823      57.65
 H       1.731443     2.591372    -3.145039      21.61
 C       2.982622     1.633047     0.165330      78.60
 H       3.372456     2.173402     1.023913      25.90
 C       3.691817     0.341206    -0.270531     -13.41
 O       4.545056    -0.381170     0.537024     202.32
 C       4.709972     0.159088     1.875087     123.30
 H       3.842829     0.351484     2.496863      27.24
 H       5.394961     0.964188     1.778425      26.77
 H       5.030232    -0.599686     2.466223      27.49
 C       3.505900    -0.093238    -1.687402       9.19
 O       3.887451    -1.430567    -1.859674     194.19
 H       4.885689    -1.447757    -2.116072      24.38
 C       2.793662     0.813467    -2.576003      26.16
 H       2.688971     0.352549    -3.592337      21.23
 C       2.466857     2.626960    -0.930072      37.24
 C       1.615734     3.840021    -0.491199     115.90
 H       1.815974     4.689666    -1.261549      20.34
 O       1.993991     4.394824     0.780971     300.92
 H       2.640905     5.054670     0.565946      29.12
 C       0.089437     3.793329    -0.665808      76.39
 H      -0.206713     3.717155    -1.702809      19.87
 C      -0.458547     5.251080    -0.091356      87.73
 O       0.047396     6.458499    -0.756336     239.18
 H       0.162024     6.439275    -1.797886      27.74
 H       0.152872     5.295072     0.809027      22.53
 H      -1.533590     4.958533    -0.052105      23.27
 C      -1.224910    -0.739809    -0.392790      53.33
 H      -0.677066    -1.741175    -0.384431      19.15
 C      -3.203925     0.471118    -1.300443      35.13
 H      -4.253057     0.530065    -1.443615      21.93
 C      -2.563074     1.697551    -0.904506      10.48
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 O      -3.088425     2.856946    -1.003332     254.89
 C      -4.244232     3.072437    -0.089431     102.02
 H      -3.798951     2.819720     1.023187      22.98
 H      -4.364412     4.159247    -0.069992      25.27
 H      -4.943952     2.520806    -0.622790      24.37
 C      -1.327516     1.592525    -0.213417      16.10
 O      -0.700145     2.825744     0.232171     175.18
 C      -0.706909     0.451627     0.079922      42.56
 H       0.457941     0.470122     0.491262      17.87
 C      -2.429699    -0.721917    -1.075956      25.80
 C      -3.329697    -1.986073    -1.233091      81.67
 H      -4.098167    -2.020168    -1.996731      20.30
 O      -2.441708    -3.071624    -1.824050     196.41
 H      -3.136890    -3.949860    -1.741443      15.13
 C      -3.923200    -2.677367     0.078578      54.63
 H      -3.004753    -3.235565     0.750763      18.88
 O      -4.811708    -1.566728     0.667653     236.14
 H      -4.999474    -2.184938     1.606511      23.59
 C      -4.930025    -3.965715    -0.348117      96.03
 O      -4.196940    -4.978017    -1.104816     303.67
 H      -3.445660    -5.459255    -0.526224      24.96
 H      -5.793201    -3.505885    -0.922073      27.85
 H      -5.314986    -4.475150     0.433729      30.35
55
name = lig-etoh-frame_748
 C       2.321671     2.108016    -2.288695      55.93
 H       1.715469     2.609459    -2.992086      20.79
 C       3.058551     1.565073     0.138395      63.18
 H       3.049836     2.073554     1.152458      21.01
 C       3.737025     0.360833    -0.227707       8.25
 O       4.505749    -0.387846     0.499534     236.07
 C       4.635428     0.120526     1.848915      94.86
 H       3.663891     0.383932     2.389915      24.41
 H       5.363545     0.988581     1.771373      24.04
 H       5.043716    -0.802575     2.533007      23.17
 C       3.475407    -0.118242    -1.591287      24.08
 O       3.923172    -1.399181    -1.842821     132.33
 H       4.977237    -1.572576    -2.140905      23.56
 C       2.749270     0.793481    -2.561249      44.70
 H       2.731258     0.144308    -3.510502      22.30
 C       2.495528     2.537236    -0.865367      50.67
 C       1.578389     3.894541    -0.496681     107.30
 H       2.084612     4.513439    -1.371532      24.26
 O       2.060472     4.387847     0.825135     284.60
 H       2.689387     5.093780     0.632152      29.58
 C       0.046339     3.856158    -0.650225      73.59
 H      -0.142514     3.583276    -1.749323      19.64
 C      -0.447866     5.285250    -0.147060     107.92
 O       0.042122     6.440556    -0.730820     285.34
 H      -0.068695     6.362123    -1.677972      32.20
 H      -0.131046     5.180247     0.925310      23.74
 H      -1.507806     4.999668    -0.265825      23.10
 C      -1.213477    -0.735440    -0.452413      26.71
 H      -0.771058    -1.687437    -0.315894      19.84
 C      -3.208794     0.470285    -1.340162      37.38
 H      -4.340734     0.365674    -1.322292      20.79
 C      -2.517683     1.659832    -0.910452       9.48
 O      -3.131919     2.848368    -1.061853     238.15
 C      -4.252810     3.080982     0.037464      86.76
 H      -3.978332     2.644121     0.891904      26.79
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 H      -4.156218     4.143212    -0.417525      21.58
 H      -5.018254     2.445203    -0.730723      21.18
 C      -1.316277     1.603652    -0.245272      -0.79
 O      -0.731109     2.805822     0.192305     176.90
 C      -0.585818     0.414796     0.196345      26.41
 H       0.400408     0.645454     0.313974      17.92
 C      -2.547838    -0.700796    -1.105894      30.88
 C      -3.284955    -1.920795    -1.254191      78.61
 H      -4.183613    -1.918766    -1.954276      21.18
 O      -2.415191    -3.129847    -1.884055     224.57
 H      -3.006069    -3.794367    -1.870201      23.18
 C      -3.906940    -2.649397     0.060237      81.57
 H      -3.248334    -3.106763     0.647552      23.92
 O      -4.819133    -1.591788     0.643023     319.28
 H      -5.184587    -1.882639     1.405020      31.71
 C      -4.930405    -3.886222    -0.334203      93.67
 O      -4.246582    -4.991519    -1.127820     304.56
 H      -3.523077    -5.258510    -0.578610      28.69
 H      -5.779899    -3.799355    -1.034450      25.67
 H      -5.476810    -4.640228     0.581848      24.46
55
name = lig-etoh-frame_749
 C       2.376689     2.053317    -2.244543      26.67
 H       1.720019     2.795687    -2.891293      13.19
 C       3.121070     1.589346     0.087764      66.79
 H       2.800686     1.732654     1.136002      16.93
 C       3.711888     0.430560    -0.279609      14.54
 O       4.481555    -0.423341     0.508817     258.65
 C       4.585078     0.058021     1.863804     110.14
 H       3.606546     0.433098     2.083956      26.09
 H       5.213802     0.933824     1.983136      26.93
 H       5.105476    -0.723075     2.327702      26.10
 C       3.440361    -0.073549    -1.488982      17.93
 O       3.954588    -1.379294    -1.855445     246.61
 H       4.840870    -1.516209    -1.925484      28.05
 C       2.761311     0.690932    -2.523183      59.68
 H       2.598957     0.286867    -3.493101      27.49
 C       2.468473     2.402147    -0.821787      92.22
 C       1.640822     3.887196    -0.500164     100.66
 H       2.023763     4.514210    -1.319444      29.11
 O       2.101003     4.373900     0.851918     247.99
 H       2.869418     5.070730     0.779950      30.06
 C       0.020101     3.896042    -0.653336      71.58
 H      -0.162857     3.594355    -1.637874      20.13
 C      -0.474248     5.232974    -0.173895     102.54
 O       0.042334     6.444479    -0.707423     239.99
 H      -0.194278     6.195908    -1.698577      28.47
 H      -0.578687     5.303407     0.939823      24.08
 H      -1.591459     5.425991    -0.414541      21.35
 C      -1.205742    -0.722354    -0.485993      18.52
 H      -0.814888    -1.762045    -0.275095      18.60
 C      -3.214363     0.496824    -1.337186      45.11
 H      -4.281723     0.391544    -1.501132      21.41
 C      -2.503391     1.583319    -0.928495       5.37
 O      -3.171806     2.870130    -1.116396     192.81
 C      -4.256672     3.080254     0.009581      95.66
 H      -4.146641     2.490563     1.083544      22.64
 H      -4.392176     4.213931    -0.111953      24.26
 H      -5.201525     2.660245    -0.184767      26.37
 C      -1.235609     1.632862    -0.250442      -3.30
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 O      -0.739212     2.822302     0.167625     178.79
 C      -0.547979     0.374900     0.198807      14.33
 H       0.613493     0.606772     0.411113      14.84
 C      -2.592913    -0.698100    -1.094355      21.01
 C      -3.264732    -2.001287    -1.290557      75.86
 H      -4.087560    -1.620149    -1.883588      22.45
 O      -2.378234    -3.132227    -1.932716     180.35
 H      -3.105221    -3.978173    -2.039134      14.84
 C      -3.988612    -2.604135     0.002890      70.06
 H      -3.140262    -2.936168     0.887461      18.23
 O      -4.801801    -1.623386     0.598206     299.56
 H      -5.341870    -1.745589     1.500451      26.51
 C      -4.931794    -3.868158    -0.323548      98.79
 O      -4.290071    -4.991698    -1.146834     292.39
 H      -3.499403    -5.281443    -0.559468      25.70
 H      -5.764057    -3.681698    -1.066308      26.67
 H      -5.300965    -4.137150     0.609109      29.13
55
name = lig-etoh-frame_750
 C       2.417405     1.974998    -2.149891      38.31
 H       2.007080     2.646645    -2.800341      16.05
 C       3.132851     1.673601     0.093599      98.58
 H       2.840071     1.611306     1.120062      18.70
 C       3.715691     0.458422    -0.305875       9.25
 O       4.461847    -0.448860     0.522187     229.25
 C       4.549470     0.014415     1.867781      98.21
 H       3.461760     0.253008     2.194769      24.81
 H       5.152028     0.952206     2.085498      26.06
 H       5.050766    -0.862976     2.457976      24.58
 C       3.425314    -0.075232    -1.521341      19.35
 O       3.931558    -1.343840    -1.875169     192.10
 H       5.043581    -1.387720    -1.579967      21.05
 C       2.781313     0.617161    -2.471721      58.15
 H       2.468780     0.372025    -3.569246      23.41
 C       2.381372     2.338174    -0.839814      74.70
 C       1.752215     3.814256    -0.463511      96.40
 H       1.911735     4.702794    -1.297155      20.03
 O       2.115909     4.357588     0.854849     282.51
 H       3.001610     4.754795     0.872755      31.55
 C       0.037843     3.885511    -0.636918      61.43
 H      -0.265927     3.725180    -1.758059      16.36
 C      -0.610984     5.202781    -0.163970     102.89
 O       0.059242     6.447536    -0.707637     235.86
 H       0.061960     6.345588    -1.709875      31.14
 H      -0.669518     5.395711     0.885930      25.34
 H      -1.567840     5.456579    -0.543991      23.50
 C      -1.214953    -0.728706    -0.479816      48.55
 H      -0.859036    -1.744561    -0.337302      20.96
 C      -3.228801     0.486641    -1.319083      24.52
 H      -4.223650     0.661792    -1.822164      19.96
 C      -2.495870     1.604958    -0.929687     -11.11
 O      -3.227205     2.877100    -1.134075     200.43
 C      -4.259979     3.065929    -0.031315     105.00
 H      -3.929969     2.762232     0.899304      26.34
 H      -4.536353     4.198452     0.380095      24.06
 H      -5.470935     2.827496     0.055544      23.59
 C      -1.143153     1.621940    -0.251630       6.53
 O      -0.721849     2.880821     0.168393     205.75
 C      -0.550445     0.385646     0.088027      43.77
 H       0.385876     0.197268     0.634144      18.96
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 C      -2.510563    -0.738581    -1.037225      16.42
 C      -3.267410    -2.124632    -1.330689      70.70
 H      -4.028266    -1.669319    -2.052966      21.22
 O      -2.379259    -3.111827    -1.967122     269.36
 H      -2.971215    -3.886728    -2.149283      19.88
 C      -4.042343    -2.608963    -0.021076      99.42
 H      -3.307068    -2.729691     0.633213      23.16
 O      -4.807497    -1.613188     0.538507     297.72
 H      -5.149873    -1.929190     1.539527      24.47
 C      -4.907826    -3.835364    -0.369427      61.54
 O      -4.320889    -4.979267    -1.132055     319.53
 H      -3.563806    -5.451263    -0.630458      26.09
 H      -5.736606    -3.337188    -0.893631      27.60
 H      -5.285317    -3.977018     0.887150      25.30
55
name = lig-etoh-frame_751
 C       2.432799     1.864811    -2.080997      53.42
 H       2.185073     2.533585    -3.030374      16.85
 C       3.132759     1.707057     0.144179      90.41
 H       3.049063     1.896797     1.285954      16.76
 C       3.741377     0.466640    -0.276142       3.01
 O       4.439117    -0.448022     0.526624     241.95
 C       4.507723    -0.037018     1.908103     122.77
 H       3.565495    -0.052853     2.457060      26.99
 H       5.064776     0.886339     2.012335      27.83
 H       4.823664    -0.873993     2.558485      25.84
 C       3.458959    -0.151984    -1.607455      13.99
 O       3.923279    -1.308639    -1.892088     169.96
 H       4.733268    -1.421672    -1.389256      23.95
 C       2.754102     0.629343    -2.487876      69.08
 H       2.573754     0.251312    -3.420739      24.14
 C       2.282751     2.397532    -0.829834      77.84
 C       1.816961     3.757314    -0.437162     100.34
 H       2.037496     4.514999    -1.145626      22.74
 O       2.115059     4.321286     0.844519     290.93
 H       3.140002     4.348896     0.910122      29.14
 C       0.069852     3.848522    -0.619971      76.20
 H      -0.168345     3.824008    -1.632189      20.31
 C      -0.735817     5.234204    -0.176700      76.93
 O       0.089443     6.448193    -0.704184     226.83
 H       0.308415     6.391065    -1.663366      31.16
 H      -0.575085     5.360187     0.953645      23.62
 H      -1.790271     5.058458    -0.644062      22.28
 C      -1.240233    -0.768567    -0.451347      59.29
 H      -0.743328    -1.737284    -0.332323      20.08
 C      -3.200356     0.456507    -1.285853      28.67
 H      -3.959391     0.780315    -2.035546      17.19
 C      -2.489193     1.679129    -0.910286     -27.68
 O      -3.301341     2.879223    -1.123771     203.89
 C      -4.296072     3.092875    -0.042440     101.26
 H      -3.532590     2.650973     0.802015      21.96
 H      -4.258878     4.133058     0.329655      25.07
 H      -5.218646     2.688926    -0.279263      26.96
 C      -1.106541     1.637625    -0.276304       0.68
 O      -0.688903     2.937373     0.191965     219.05
 C      -0.567187     0.393597    -0.055150      53.77
 H       0.158371     0.015630     0.738629      18.04
 C      -2.454890    -0.807819    -1.004885      18.84
 C      -3.277650    -2.169853    -1.381930      81.58
 H      -3.968147    -2.066157    -2.232195      21.73
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 O      -2.385840    -3.080136    -1.988349     280.30
 H      -2.900241    -3.869840    -2.197183      23.11
 C      -4.030544    -2.637833    -0.098191      81.80
 H      -3.064700    -2.914282     0.668983      19.31
 O      -4.848376    -1.578201     0.494640     323.53
 H      -4.831650    -1.969065     1.313233      27.29
 C      -4.889142    -3.799569    -0.352012     104.79
 O      -4.362075    -4.954088    -1.103014     367.15
 H      -3.734734    -5.453531    -0.596238      32.13
 H      -5.787426    -3.280596    -0.810561      27.13
 H      -5.268963    -4.211517     0.508114      29.45
55
name = lig-etoh-frame_752
 C       2.369847     1.862441    -2.101263      76.81
 H       2.194415     2.389147    -2.977303      18.33
 C       3.113382     1.691252     0.204245      62.81
 H       3.345878     2.222693     1.107596      19.57
 C       3.734607     0.468892    -0.263813       4.77
 O       4.414541    -0.439002     0.546587     228.72
 C       4.459503    -0.112582     1.973533     101.82
 H       3.447644    -0.059343     2.508173      25.06
 H       5.018078     0.846762     2.048160      24.98
 H       5.027635    -0.972350     2.498836      24.65
 C       3.490801    -0.132812    -1.605645      22.97
 O       3.919379    -1.345009    -1.928112     136.40
 H       4.656848    -1.639785    -1.294360      22.50
 C       2.747820     0.597446    -2.514997      56.16
 H       2.664432     0.130800    -3.583446      21.74
 C       2.270814     2.443267    -0.745945      63.34
 C       1.770995     3.746224    -0.424740      87.49
 H       2.364096     4.434413    -1.308988      22.57
 O       2.130107     4.268092     0.840408     304.86
 H       3.096399     3.991688     1.021231      27.06
 C       0.115433     3.855105    -0.574471      72.00
 H      -0.024035     3.657546    -1.722848      18.93
 C      -0.767994     5.269192    -0.222567      86.82
 O       0.092865     6.441270    -0.675755     228.81
 H       0.333645     6.152148    -1.681554      27.21
 H      -0.701760     5.300917     0.828409      25.76
 H      -1.723552     4.856527    -0.483628      23.48
 C      -1.242535    -0.847816    -0.418858      29.55
 H      -0.576429    -1.730749    -0.213375      18.80
 C      -3.078095     0.455126    -1.244741      35.78
 H      -3.841288     0.512954    -2.022047      18.73
 C      -2.496311     1.726231    -0.885994      -2.75
 O      -3.346809     2.878483    -1.131670     229.21
 C      -4.237605     3.094525    -0.021770      85.04
 H      -3.909798     2.338604     0.681452      24.52
 H      -4.179818     4.311065    -0.000033      21.64
 H      -5.116807     2.442328    -0.551401      21.80
 C      -1.154136     1.722086    -0.326211      -7.22
 O      -0.648919     2.948050     0.231817     218.58
 C      -0.568475     0.383753    -0.167224      22.67
 H       0.163024     0.278265     0.739266      17.26
 C      -2.534491    -0.866164    -1.051532      16.04
 C      -3.286444    -2.144246    -1.440425      89.23
 H      -4.080056    -2.109925    -2.229065      21.26
 O      -2.357816    -3.070405    -1.999559     218.95
 H      -2.907326    -4.032422    -2.200337      17.40
 C      -3.919184    -2.658939    -0.161175     111.25
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 H      -3.243959    -3.038790     0.475926      24.39
 O      -4.879388    -1.556410     0.440010     257.58
 H      -4.624650    -1.829796     1.542417      22.31
 C      -4.912942    -3.796589    -0.351559      99.64
 O      -4.409529    -4.917312    -1.094001     291.10
 H      -3.810183    -5.415259    -0.403684      26.96
 H      -5.795067    -3.552044    -0.930990      26.02
 H      -5.407004    -4.495623     0.643946      24.84
55
name = lig-etoh-frame_753
 C       2.258818     1.915386    -2.119870      82.67
 H       1.870173     2.627769    -2.968261      17.07
 C       3.080199     1.664410     0.219649      76.32
 H       3.670370     2.303404     0.973183      23.27
 C       3.697403     0.463413    -0.260329      15.33
 O       4.391182    -0.433025     0.585166     224.20
 C       4.423165    -0.195397     2.046032     105.33
 H       3.412342    -0.031382     2.358683      25.61
 H       4.933871     0.772569     2.255426      24.47
 H       5.253848    -0.926131     2.263551      24.16
 C       3.511837    -0.062978    -1.535234      21.35
 O       3.921342    -1.416498    -1.972691     184.10
 H       4.629690    -1.914584    -1.259010      20.38
 C       2.766118     0.544658    -2.541316      34.88
 H       2.722005     0.294383    -3.569816      26.81
 C       2.342379     2.374362    -0.698422      58.62
 C       1.694210     3.811831    -0.441940     107.05
 H       2.208537     4.341411    -1.227306      26.37
 O       2.146084     4.206301     0.856346     348.96
 H       2.992068     3.917346     1.083337      27.81
 C       0.160416     3.902273    -0.570810      79.31
 H       0.059779     3.473570    -1.532142      20.93
 C      -0.675945     5.259727    -0.263319      90.36
 O       0.059698     6.406684    -0.666245     274.67
 H       0.162488     6.129025    -1.553680      32.14
 H      -0.856090     5.331754     0.882430      23.18
 H      -1.781135     5.086276    -0.620620      21.66
 C      -1.235094    -0.915348    -0.405147      10.41
 H      -0.654311    -1.754225    -0.096993      19.44
 C      -2.951483     0.446249    -1.239334      42.32
 H      -3.927493     0.287043    -1.805248      20.88
 C      -2.503448     1.751558    -0.873652      24.03
 O      -3.317927     2.856890    -1.164593     255.23
 C      -4.209090     3.048599    -0.051910     119.28
 H      -4.273029     2.387718     0.978800      23.33
 H      -4.468669     4.155545    -0.088792      24.89
 H      -5.173015     2.757308    -0.375390      26.86
 C      -1.233997     1.795722    -0.376861       0.72
 O      -0.605841     2.912057     0.278615     200.52
 C      -0.587374     0.408379    -0.222822      -1.01
 H       0.306727     0.585826     0.412093      17.91
 C      -2.590545    -0.876507    -1.102175      13.80
 C      -3.303139    -2.103931    -1.505202      87.24
 H      -4.171015    -1.792631    -2.107975      23.78
 O      -2.316818    -3.102767    -2.014056     260.52
 H      -2.798430    -3.861246    -2.037411      23.97
 C      -3.894026    -2.670667    -0.202331      82.57
 H      -3.054972    -3.069662     0.610638      19.09
 O      -4.855938    -1.575321     0.422884     332.20
 H      -4.754511    -1.407048     1.327545      29.23
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 C      -4.996337    -3.852565    -0.339302      98.97
 O      -4.424006    -4.909157    -1.093894     347.33
 H      -3.833446    -5.397565    -0.473142      29.70
 H      -5.864760    -3.616694    -1.027455      26.58
 H      -5.294418    -4.053628     0.644869      29.02
55
name = lig-etoh-frame_754
 C       2.157932     1.929837    -2.132770      30.36
 H       1.528513     2.648392    -2.647376      14.56
 C       3.096797     1.636443     0.224469      82.64
 H       3.713836     2.057115     0.962292      26.60
 C       3.662932     0.434198    -0.207794      28.67
 O       4.372277    -0.421978     0.620969     226.23
 C       4.429322    -0.239118     2.068573     106.46
 H       3.326761    -0.312210     2.460806      24.26
 H       4.833096     0.723812     2.433036      24.66
 H       5.101755    -1.030827     2.371362      25.59
 C       3.529565    -0.079410    -1.514882      18.01
 O       3.915107    -1.465862    -1.990077     236.45
 H       4.511123    -1.802852    -1.435652      26.13
 C       2.767355     0.622117    -2.521360      37.16
 H       2.759098     0.319115    -3.604296      26.96
 C       2.370246     2.319151    -0.765503      72.74
 C       1.663382     3.833435    -0.414884     111.16
 H       1.999513     4.638639    -1.338400      23.04
 O       2.129438     4.170316     0.890315     295.03
 H       3.102197     3.925915     1.021772      25.21
 C       0.167964     3.929494    -0.565797      66.57
 H      -0.045148     3.507137    -1.602949      17.32
 C      -0.583532     5.205306    -0.262748     112.64
 O       0.018242     6.377816    -0.670558     222.68
 H       0.103705     6.366269    -1.732320      27.90
 H      -0.807444     5.310091     0.767661      25.08
 H      -1.466023     5.408227    -0.843571      21.94
 C      -1.228311    -0.896321    -0.416326      30.79
 H      -0.796050    -1.882776    -0.016825      18.64
 C      -2.937924     0.424724    -1.292471      42.05
 H      -3.992775     0.532905    -1.527121      25.00
 C      -2.517333     1.744459    -0.896171      21.87
 O      -3.266278     2.822833    -1.178450     253.86
 C      -4.269915     2.996878    -0.085984     115.33
 H      -4.144071     2.851252     0.980794      25.47
 H      -4.516468     4.157845     0.141464      24.76
 H      -5.441582     2.872443    -0.365920      24.35
 C      -1.250429     1.808280    -0.387790      10.28
 O      -0.563555     2.854399     0.319147     152.94
 C      -0.644996     0.445767    -0.238510       8.62
 H       0.536461     0.664153    -0.125266      16.80
 C      -2.495974    -0.856271    -1.093533      19.18
 C      -3.310698    -2.069361    -1.533151      69.65
 H      -4.079878    -1.647403    -2.215721      22.25
 O      -2.290002    -3.109549    -2.025224     196.48
 H      -2.863408    -4.013893    -1.909397      16.37
 C      -3.952159    -2.690438    -0.171559      97.05
 H      -3.118670    -2.843553     0.429447      21.66
 O      -4.810799    -1.603138     0.374204     377.74
 H      -4.698033    -1.261630     1.308362      27.72
 C      -5.050958    -3.849999    -0.368909      66.13
 O      -4.419908    -4.942670    -1.096294     336.80
 H      -3.743356    -5.447633    -0.615218      28.96
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 H      -5.903456    -3.435635    -0.887718      27.31
 H      -5.357341    -3.850597     0.915538      23.29
55
name = lig-etoh-frame_755
 C       2.089562     1.887151    -2.100715      19.61
 H       1.309928     2.459342    -2.629470      21.07
 C       3.136710     1.607648     0.190016      54.36
 H       3.515318     1.972086     1.231765      18.97
 C       3.638473     0.360683    -0.150208      31.29
 O       4.372609    -0.417624     0.662676     257.03
 C       4.408798    -0.274922     2.083725     123.01
 H       3.514953    -0.620005     2.572440      27.24
 H       4.761151     0.695337     2.505946      25.86
 H       4.874503    -1.215214     2.604540      24.48
 C       3.514058    -0.146748    -1.570805      39.64
 O       3.873489    -1.450866    -2.000435     121.20
 H       4.735617    -1.724543    -1.400458      22.12
 C       2.767166     0.759021    -2.481795      50.60
 H       2.743946     0.254109    -3.474285      19.53
 C       2.340682     2.352106    -0.858123      54.91
 C       1.694334     3.823238    -0.401369     108.98
 H       1.908980     4.675706    -1.106563      20.52
 O       2.101965     4.149644     0.935644     279.95
 H       3.123628     4.127094     0.817034      27.21
 C       0.141252     3.875610    -0.569244      77.58
 H      -0.141046     3.776783    -1.624835      19.02
 C      -0.529380     5.157796    -0.270198     100.45
 O       0.033706     6.408181    -0.701508     230.15
 H       0.018098     6.552320    -1.691196      30.42
 H      -0.712291     5.234703     0.846360      23.82
 H      -1.479138     5.118667    -0.908711      21.89
 C      -1.203802    -0.820437    -0.429877      60.07
 H      -0.847850    -1.751510    -0.107912      19.53
 C      -3.020148     0.450397    -1.361025      37.74
 H      -4.107687     0.695676    -1.468244      21.42
 C      -2.503584     1.681098    -0.941883       6.46
 O      -3.263260     2.817549    -1.158130     235.45
 C      -4.395922     3.041820    -0.133861      96.85
 H      -3.771264     2.686234     0.840579      22.02
 H      -4.198243     4.117244     0.116538      23.32
 H      -5.341319     2.583462    -0.452502      24.89
 C      -1.202481     1.752073    -0.347902      15.86
 O      -0.525724     2.796392     0.335545     167.69
 C      -0.651170     0.485057    -0.249938      45.90
 H       0.370893     0.425632    -0.354122      20.30
 C      -2.365473    -0.838841    -1.070954      20.87
 C      -3.284661    -2.046275    -1.510968      64.19
 H      -3.886956    -1.804786    -2.420554      20.90
 O      -2.308321    -3.111467    -2.028354     217.16
 H      -2.800760    -4.031655    -1.835910      17.18
 C      -4.065845    -2.662574    -0.175070      82.95
 H      -3.085659    -2.882433     0.488442      18.39
 O      -4.775075    -1.621909     0.312266     344.40
 H      -4.391185    -1.405543     1.343052      23.15
 C      -5.039218    -3.804492    -0.335451      89.58
 O      -4.433694    -4.990021    -1.102528     323.39
 H      -3.622093    -5.410334    -0.571285      26.37
 H      -5.943170    -3.357191    -0.840127      25.60
 H      -5.418868    -4.091495     0.603475      27.33
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name = lig-etoh-frame_756
 C       2.015499     1.860480    -2.071349      67.84
 H       1.260012     2.131628    -2.886767      23.68
 C       3.161326     1.616355     0.126157      51.91
 H       2.996124     1.937653     1.140876      18.07
 C       3.607219     0.277424    -0.167568      19.33
 O       4.400658    -0.447578     0.717861     237.29
 C       4.375774    -0.347322     2.141383     122.29
 H       3.324730    -0.588975     2.585846      26.83
 H       4.738606     0.610702     2.493478      27.05
 H       5.023302    -1.124112     2.487646      26.87
 C       3.455953    -0.159115    -1.607964      32.27
 O       3.833491    -1.409933    -1.985860     149.99
 H       4.877586    -1.543984    -1.715613      21.16
 C       2.812393     0.777427    -2.448901      38.19
 H       2.596338     0.355046    -3.414440      20.10
 C       2.319090     2.450188    -0.831294      53.01
 C       1.712279     3.759247    -0.397844     105.56
 H       2.124577     4.760739    -0.982839      17.65
 O       2.086204     4.133907     0.972884     290.00
 H       2.975640     4.444424     0.872132      29.84
 C       0.141415     3.774971    -0.574629      85.20
 H      -0.095523     3.684547    -1.647907      20.44
 C      -0.544473     5.146598    -0.272561      93.96
 O       0.074301     6.466412    -0.721584     241.73
 H      -0.049623     6.406424    -1.684494      30.08
 H      -0.605426     5.240687     0.818853      25.72
 H      -1.543952     4.733826    -0.561707      23.26
 C      -1.165481    -0.728249    -0.440274      51.71
 H      -0.555585    -1.667521    -0.201895      18.30
 C      -3.110353     0.478320    -1.401362      30.26
 H      -4.163291     0.437946    -1.692831      21.21
 C      -2.476385     1.636371    -0.982206       4.80
 O      -3.284510     2.834304    -1.140371     224.09
 C      -4.407636     3.081791    -0.147287      86.94
 H      -3.980479     2.271138     0.448948      23.18
 H      -4.302542     4.199444    -0.103001      23.05
 H      -5.322760     2.410776    -0.477090      23.70
 C      -1.171385     1.678958    -0.297510      22.38
 O      -0.491447     2.754242     0.314410     204.00
 C      -0.588156     0.485816    -0.248493      44.49
 H       0.612643     0.247028    -0.169300      16.66
 C      -2.390486    -0.800621    -1.109217      14.87
 C      -3.210317    -2.066006    -1.474962      80.44
 H      -3.772200    -1.906096    -2.400834      20.33
 O      -2.342950    -3.117699    -2.011423     295.29
 H      -2.744222    -3.904547    -1.871686      26.00
 C      -4.085453    -2.634776    -0.224978     107.52
 H      -3.373095    -3.072917     0.464698      21.84
 O      -4.759564    -1.586691     0.310788     433.55
 H      -4.381185    -1.610097     1.108565      32.26
 C      -5.008737    -3.791289    -0.350286      95.44
 O      -4.450754    -5.025179    -1.094536     311.00
 H      -3.742278    -5.256370    -0.510823      30.25
 H      -5.871449    -3.536332    -0.953049      24.90
 H      -5.500414    -4.430805     0.711053      23.53
55
name = lig-etoh-frame_757
 C       1.968396     1.848374    -2.052303      87.88
 H       1.402054     2.060243    -2.895561      24.46
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 C       3.128804     1.637363     0.036633      64.44
 H       2.746218     1.931814     1.047637      18.97
 C       3.574623     0.248979    -0.219092      13.37
 O       4.427053    -0.500153     0.743600     202.67
 C       4.316448    -0.418766     2.214805     109.60
 H       3.299576    -0.425019     2.504174      26.47
 H       4.700054     0.613614     2.510975      24.96
 H       5.274141    -1.074217     2.377744      23.57
 C       3.407371    -0.125898    -1.559551      42.81
 O       3.816449    -1.373859    -1.988468     226.39
 H       4.769233    -1.521571    -2.016409      25.74
 C       2.835677     0.718748    -2.443733      14.15
 H       2.481100     0.469453    -3.499354      18.75
 C       2.324058     2.496202    -0.774048      42.45
 C       1.722163     3.732676    -0.380328     113.50
 H       2.189153     4.515820    -1.023646      19.08
 O       2.065630     4.112658     1.010147     270.36
 H       2.855562     4.781828     1.081650      25.70
 C       0.180388     3.702591    -0.591904      71.71
 H       0.025061     3.274359    -1.637771      21.32
 C      -0.564612     5.132409    -0.231134      79.47
 O       0.085464     6.487472    -0.740797     213.31
 H       0.016351     6.194067    -1.794333      24.56
 H      -0.444668     5.308544     0.851583      23.40
 H      -1.678124     4.922398    -0.311277      23.34
 C      -1.151716    -0.709475    -0.482848      37.97
 H      -0.409199    -1.484494    -0.413762      19.01
 C      -3.155100     0.441337    -1.413209      38.61
 H      -4.078773     0.254816    -2.003715      18.58
 C      -2.483239     1.663911    -0.995760       6.16
 O      -3.281334     2.858563    -1.149357     237.19
 C      -4.365158     3.034642    -0.190199     101.85
 H      -4.349640     2.311740     0.761376      24.78
 H      -4.755445     4.164553    -0.071413      23.87
 H      -5.383230     2.714309    -0.634097      25.26
 C      -1.186225     1.650093    -0.275358      -4.92
 O      -0.466819     2.728837     0.271480     189.86
 C      -0.401582     0.433045    -0.217307      21.93
 H       0.505282     0.487371     0.243304      18.03
 C      -2.493287    -0.747599    -1.160191      17.02
 C      -3.136358    -2.116172    -1.450735      87.49
 H      -3.923445    -1.763208    -2.212637      21.70
 O      -2.348540    -3.118383    -1.980692     217.04
 H      -2.923529    -4.090786    -1.893746      15.66
 C      -4.036181    -2.644030    -0.301264      86.77
 H      -3.321683    -3.120908     0.536292      18.74
 O      -4.771955    -1.512282     0.334678     333.84
 H      -4.495325    -1.566191     1.367712      24.10
 C      -5.036483    -3.871595    -0.402789     102.00
 O      -4.463449    -5.032627    -1.076974     320.10
 H      -3.727985    -5.358544    -0.455610      28.26
 H      -5.910578    -3.699325    -1.065576      25.46
 H      -5.293527    -4.171225     0.574487      29.51
55
name = lig-etoh-frame_758
 C       2.017616     1.823159    -2.025320      81.96
 H       1.396798     2.397741    -2.862761      23.22
 C       3.060800     1.634689     0.004534      74.15
 H       3.037043     1.890892     1.091053      20.53
 C       3.562455     0.297287    -0.210664      33.40
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 O       4.420258    -0.547185     0.717852     207.44
 C       4.311410    -0.431518     2.240745     117.36
 H       3.228039    -0.598077     2.642599      25.52
 H       4.584821     0.559485     2.550144      26.82
 H       5.010819    -1.140731     2.596500      27.27
 C       3.418200    -0.140010    -1.490366      50.40
 O       3.784962    -1.355359    -2.004240     133.46
 H       4.881823    -1.576737    -2.230581      21.68
 C       2.743214     0.711724    -2.473920       0.95
 H       2.667728     0.357889    -3.473144      17.83
 C       2.334614     2.419167    -0.798001      51.02
 C       1.725766     3.763902    -0.316142     102.20
 H       2.162220     4.423428    -1.267300      17.97
 O       2.041057     4.093773     1.049984     296.74
 H       2.604155     4.911154     1.150905      25.65
 C       0.204352     3.672628    -0.624373      72.47
 H       0.102697     3.207604    -1.562633      21.69
 C      -0.557709     5.124433    -0.160947      77.66
 O       0.060314     6.442392    -0.784876     218.14
 H       0.213064     6.286925    -1.705203      31.01
 H      -0.188418     5.255567     0.901285      21.72
 H      -1.620839     5.340850    -0.347670      23.33
 C      -1.134457    -0.720067    -0.567261      23.53
 H      -0.569215    -1.708087    -0.641764      19.52
 C      -3.163541     0.409554    -1.421304      42.67
 H      -3.955619     0.448784    -2.188317      19.29
 C      -2.513143     1.705169    -0.980257      -0.07
 O      -3.256637     2.886595    -1.149206     238.32
 C      -4.380987     2.962664    -0.225652     119.91
 H      -4.513039     2.846352     0.854219      25.19
 H      -4.697875     3.978396     0.056785      26.78
 H      -5.373161     2.797634    -0.903183      24.17
 C      -1.200225     1.623306    -0.293405     -13.50
 O      -0.459153     2.714207     0.243359     150.37
 C      -0.301945     0.414036    -0.178773       5.51
 H       0.539588     0.668491     0.671171      14.37
 C      -2.507740    -0.743201    -1.159123      21.95
 C      -3.154886    -2.117610    -1.448084      96.32
 H      -3.982334    -1.769856    -2.058096      23.37
 O      -2.338095    -3.167470    -1.949356     277.67
 H      -2.944127    -3.899129    -1.964647      23.04
 C      -3.977647    -2.668659    -0.294619      75.62
 H      -3.232200    -2.942039     0.451735      20.38
 O      -4.766055    -1.450312     0.369500     281.39
 H      -4.857387    -1.539302     1.441972      24.70
 C      -5.056356    -3.923661    -0.522419      66.63
 O      -4.448860    -5.048697    -1.054872     323.59
 H      -3.748706    -5.580485    -0.540517      27.37
 H      -6.009854    -3.691972    -1.036931      26.60
 H      -5.335715    -3.986408     0.844187      23.29
55
name = lig-etoh-frame_759
 C       2.077215     1.841367    -2.078495      55.04
 H       1.594442     2.585865    -2.584961      21.15
 C       3.036034     1.581197     0.105022      65.90
 H       3.469721     1.972723     1.042547      21.70
 C       3.588647     0.353077    -0.147228      39.02
 O       4.379452    -0.571323     0.685799     227.55
 C       4.277636    -0.424314     2.226767     112.53
 H       3.375872    -0.822901     2.646402      26.51
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 H       4.548390     0.605690     2.618547      24.56
 H       4.785342    -1.306181     2.832888      24.37
 C       3.431313    -0.152249    -1.498346      61.47
 O       3.776565    -1.371759    -2.039276     197.81
 H       4.665480    -1.488956    -2.032250      24.88
 C       2.634134     0.681199    -2.470762      48.84
 H       2.821276     0.206335    -3.479089      24.07
 C       2.313755     2.338502    -0.827517      44.64
 C       1.733798     3.783077    -0.303839     109.43
 H       2.062000     4.536477    -1.036645      20.67
 O       2.008484     4.078333     1.081053     330.71
 H       2.433151     4.904576     1.076601      29.01
 C       0.184511     3.699624    -0.619499      71.76
 H       0.073969     3.477883    -1.773151      17.82
 C      -0.483735     5.142663    -0.128544      88.58
 O       0.032887     6.376041    -0.800406     225.93
 H       0.294144     6.248380    -1.811822      26.59
 H      -0.165582     5.141023     0.890093      22.81
 H      -1.546703     5.391482    -0.357044      22.47
 C      -1.076415    -0.763634    -0.655553      41.93
 H      -0.930741    -1.855457    -0.718344      21.85
 C      -3.137018     0.469467    -1.432772      32.80
 H      -3.946083     0.688016    -2.136206      21.42
 C      -2.524669     1.687157    -0.949101      -3.96
 O      -3.214090     2.912580    -1.119016     215.53
 C      -4.470490     2.955264    -0.271441      87.74
 H      -4.316248     2.663055     0.817137      24.21
 H      -4.314124     4.167154    -0.180064      22.12
 H      -5.266974     2.536565    -1.001584      23.72
 C      -1.181917     1.594024    -0.333621      -0.99
 O      -0.472198     2.707649     0.239671     170.33
 C      -0.352721     0.421979    -0.135963      36.28
 H       0.399809     0.447128     0.561930      18.50
 C      -2.425748    -0.791075    -1.125200       5.53
 C      -3.230099    -2.065630    -1.452510      77.75
 H      -3.978863    -1.915040    -2.317658      21.00
 O      -2.317106    -3.212394    -1.923688     212.68
 H      -2.972813    -3.981302    -2.032127      20.29
 C      -3.966089    -2.661637    -0.217501      69.99
 H      -3.143727    -2.974514     0.535448      18.77
 O      -4.752758    -1.420440     0.393194     319.94
 H      -4.984739    -1.702122     1.212517      29.43
 C      -5.047224    -3.913269    -0.531785     100.61
 O      -4.428367    -5.100844    -1.061180     354.76
 H      -3.787990    -5.527643    -0.497522      31.59
 H      -5.968146    -3.632679    -1.057705      28.24
 H      -5.405524    -3.935657     0.378767      31.35
55
name = lig-etoh-frame_760
 C       2.122375     1.911083    -2.142660      40.37
 H       1.639712     2.724311    -2.835251      17.50
 C       3.049147     1.546521     0.270335      67.01
 H       3.656092     2.228594     0.945815      24.81
 C       3.639715     0.318515    -0.124917       9.10
 O       4.324829    -0.572383     0.685149     208.84
 C       4.242912    -0.442726     2.204953     102.79
 H       3.143737    -0.735613     2.461825      25.17
 H       4.517147     0.511961     2.599584      25.49
 H       4.909553    -1.177763     2.612463      25.97
 C       3.391726    -0.115798    -1.537660      24.68
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 O       3.762231    -1.396386    -2.068314     152.58
 H       4.810634    -1.556332    -1.738649      21.52
 C       2.601384     0.563187    -2.448556      41.16
 H       2.672304     0.245979    -3.490869      27.77
 C       2.299353     2.305248    -0.767369      53.81
 C       1.720068     3.734688    -0.339723      94.37
 H       2.122388     4.854770    -0.718093      19.93
 O       1.972281     4.054483     1.098591     268.82
 H       2.410881     4.971092     1.054379      26.56
 C       0.139689     3.779189    -0.610134      85.91
 H      -0.053943     3.816029    -1.631204      20.10
 C      -0.396627     5.155523    -0.151214     101.52
 O       0.035639     6.318629    -0.806810     280.83
 H       0.102066     6.001749    -1.769499      28.86
 H      -0.264676     5.203784     1.000861      21.82
 H      -1.506825     4.954807    -0.206075      23.02
 C      -1.044279    -0.834909    -0.722986      48.11
 H      -0.726049    -1.879977    -0.523385      21.66
 C      -3.054196     0.543906    -1.423002      39.30
 H      -4.049909     0.663518    -1.924937      22.86
 C      -2.503246     1.642001    -0.917251       1.39
 O      -3.150631     2.912819    -1.072501     200.94
 C      -4.500088     3.017791    -0.319710      88.59
 H      -4.214252     2.225229     0.449367      22.03
 H      -4.470871     4.044447    -0.434858      24.64
 H      -5.377046     2.379024    -0.863355      24.54
 C      -1.135736     1.585336    -0.363521      17.11
 O      -0.500451     2.712909     0.235588     165.61
 C      -0.532833     0.384717    -0.147603      40.73
 H       0.507674     0.214052     0.406252      19.05
 C      -2.371153    -0.785758    -1.134958       2.56
 C      -3.291391    -2.042633    -1.473215      72.71
 H      -3.813899    -1.966323    -2.392779      21.38
 O      -2.306030    -3.239034    -1.891202     169.14
 H      -2.932424    -4.135502    -2.078116      17.38
 C      -3.996879    -2.612419    -0.142319      71.10
 H      -3.236271    -3.074372     0.569068      19.42
 O      -4.715510    -1.432403     0.389919     262.15
 H      -5.154784    -1.988159     1.266073      24.03
 C      -4.989777    -3.849842    -0.540852      60.52
 O      -4.421057    -5.154048    -1.082992     230.85
 H      -3.716056    -5.355666    -0.346635      25.91
 H      -5.735424    -3.540271    -1.330897      26.26
 H      -5.698253    -4.192047     0.700954      23.89
55
name = lig-etoh-frame_761
 C       2.168508     1.970369    -2.156744      38.27
 H       1.810181     2.447959    -3.045336      17.50
 C       3.082283     1.550823     0.375676      63.92
 H       3.501172     2.277621     1.030261      24.14
 C       3.657186     0.270695    -0.142636      -4.36
 O       4.284274    -0.572864     0.701061     216.23
 C       4.178737    -0.471070     2.148052      97.09
 H       3.123240    -0.497902     2.305655      26.21
 H       4.485501     0.558160     2.525822      24.38
 H       5.078364    -1.156445     2.349870      23.69
 C       3.350410    -0.121965    -1.544414      12.81
 O       3.788015    -1.409923    -2.075931     180.94
 H       4.586422    -1.761313    -1.480516      22.63
 C       2.573733     0.525948    -2.446298      40.91
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 H       2.404186     0.218404    -3.483836      24.52
 C       2.302660     2.312987    -0.695798      55.92
 C       1.702191     3.702362    -0.365129     106.07
 H       2.157433     4.566550    -0.807873      24.96
 O       1.936371     4.021548     1.107026     264.92
 H       2.421474     4.903233     1.155044      28.20
 C       0.139430     3.868578    -0.573011      63.37
 H      -0.254453     3.812555    -1.696615      19.72
 C      -0.379339     5.129735    -0.104329     112.73
 O       0.048119     6.263170    -0.822593     270.91
 H      -0.064599     6.014327    -1.801141      29.03
 H      -0.242959     5.414718     0.900545      24.28
 H      -1.413497     4.699593    -0.141340      22.40
 C      -1.059548    -0.917432    -0.747272      41.63
 H      -0.320144    -1.670303    -0.336222      20.71
 C      -2.979643     0.514061    -1.407644      52.43
 H      -4.031469     0.459134    -1.633874      23.79
 C      -2.431428     1.678218    -0.880442       6.22
 O      -3.081222     2.897342    -1.030524     217.41
 C      -4.469985     3.001798    -0.408497      95.63
 H      -4.360637     2.329448     0.447370      25.11
 H      -5.002120     4.154453    -0.281736      23.38
 H      -5.444506     2.486457    -0.796044      25.35
 C      -1.108540     1.619624    -0.375449      11.93
 O      -0.533331     2.735513     0.219493     165.81
 C      -0.662578     0.283857    -0.169356      33.36
 H       0.404578     0.252555     0.055547      21.49
 C      -2.392780    -0.763173    -1.213888      11.65
 C      -3.266017    -2.072656    -1.466795      68.56
 H      -3.923798    -1.842812    -2.392279      21.80
 O      -2.310567    -3.257167    -1.856953     242.73
 H      -2.796380    -3.980861    -1.960181      24.33
 C      -4.041788    -2.564424    -0.132447      81.56
 H      -3.284700    -2.988613     0.581891      22.15
 O      -4.684066    -1.503697     0.414956     330.53
 H      -5.236889    -1.794798     1.173699      27.96
 C      -4.974469    -3.801355    -0.491119     109.50
 O      -4.409873    -5.167856    -1.074853     297.80
 H      -3.619474    -5.334452    -0.480689      29.07
 H      -5.457022    -3.469392    -1.390665      27.84
 H      -5.536640    -4.169151     0.105433      30.76
55
name = lig-etoh-frame_762
 C       2.241549     1.924067    -2.092330      56.80
 H       1.849426     2.412545    -3.032630      17.66
 C       3.096779     1.555626     0.342446      40.34
 H       3.276772     2.081493     1.383368      18.48
 C       3.613120     0.295304    -0.161706      -0.71
 O       4.267489    -0.594681     0.687458     250.29
 C       4.147189    -0.453302     2.066822     111.29
 H       3.070991    -0.585359     2.467944      26.34
 H       4.486612     0.524136     2.385373      25.65
 H       4.842992    -1.266058     2.432313      25.13
 C       3.341715    -0.206379    -1.513381      12.32
 O       3.816177    -1.414907    -2.050441     225.60
 H       4.357985    -1.819314    -1.452876      28.41
 C       2.530677     0.618796    -2.453055      63.90
 H       2.183500     0.074124    -3.395913      23.70
 C       2.320744     2.336660    -0.670778      91.76
 C       1.682012     3.676201    -0.341639     106.46
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 H       2.321134     4.257268    -1.278848      23.06
 O       1.904688     3.984584     1.097857     289.66
 H       2.432131     4.734081     1.212465      30.91
 C       0.187809     3.868790    -0.571436      81.47
 H      -0.166963     3.660143    -1.512461      23.05
 C      -0.430991     5.114100    -0.008850      95.32
 O       0.055127     6.220599    -0.844800     243.07
 H      -0.118636     6.218063    -1.898049      25.71
 H      -0.081471     5.502682     1.017793      22.60
 H      -1.543255     5.020337    -0.138272      23.37
 C      -1.102153    -0.964075    -0.722291      46.80
 H      -0.326804    -1.670625    -0.513606      22.93
 C      -2.936824     0.432445    -1.374237      50.65
 H      -4.047253     0.368701    -1.463763      23.51
 C      -2.359508     1.737147    -0.865943       8.31
 O      -3.046367     2.909383    -0.993546     224.28
 C      -4.455454     2.980467    -0.468183     112.72
 H      -4.508598     2.741266     0.688849      24.10
 H      -4.882058     3.835210    -0.141893      27.14
 H      -5.342247     2.484098    -1.197387      24.03
 C      -1.114862     1.646251    -0.371633      14.80
 O      -0.552177     2.771425     0.210832     182.76
 C      -0.685948     0.236766    -0.215159      28.31
 H       0.405702     0.335895     0.035396      21.47
 C      -2.427167    -0.824970    -1.316023      21.35
 C      -3.207547    -2.116116    -1.466083      87.17
 H      -4.022023    -1.867742    -2.127878      24.79
 O      -2.313453    -3.222849    -1.816385     189.60
 H      -2.982287    -4.122854    -1.832575      15.28
 C      -4.030016    -2.586113    -0.159246      83.11
 H      -3.161282    -2.837312     0.578145      22.40
 O      -4.690901    -1.537644     0.449374     347.53
 H      -5.223993    -1.676094     1.209194      30.45
 C      -4.921429    -3.756545    -0.536376      65.71
 O      -4.382077    -5.139425    -1.049327     232.22
 H      -3.536703    -5.491221    -0.675954      25.88
 H      -5.476506    -3.366697    -1.451605      24.80
 H      -5.984895    -4.226551     0.300832      22.85
55
name = lig-etoh-frame_763
 C       2.291437     1.875741    -2.001081      31.42
 H       1.781862     2.650734    -2.624262      17.64
 C       3.075938     1.579717     0.243034      65.49
 H       2.979635     1.566292     1.297854      20.07
 C       3.547324     0.325791    -0.184961      27.09
 O       4.257071    -0.629876     0.631470     272.97
 C       4.111362    -0.436210     2.027823     126.03
 H       3.193423    -0.704938     2.541296      27.07
 H       4.562849     0.535678     2.355970      26.19
 H       4.564852    -1.299880     2.626530      25.32
 C       3.309560    -0.255659    -1.491675      12.39
 O       3.820884    -1.401403    -2.024828     162.23
 H       4.391085    -1.977485    -1.230639      22.55
 C       2.543746     0.644647    -2.418118      76.20
 H       2.148747     0.205791    -3.268901      25.10
 C       2.363374     2.331959    -0.660905      79.94
 C       1.710282     3.663005    -0.335834     122.60
 H       2.179103     4.200730    -1.115767      26.03
 O       1.882632     3.949941     1.058244     284.17
 H       2.597236     4.664056     1.207802      27.50
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 C       0.215270     3.798388    -0.544574      67.79
 H      -0.005791     3.621933    -1.691932      19.26
 C      -0.488957     5.152517     0.051853      96.05
 O       0.062239     6.219435    -0.838930     273.48
 H      -0.051684     6.036849    -1.793804      28.38
 H      -0.058128     5.281600     1.024343      24.23
 H      -1.543316     5.311814    -0.023568      24.66
 C      -1.159126    -0.962794    -0.690100      21.95
 H      -0.605609    -1.977847    -0.836354      18.39
 C      -2.954282     0.400757    -1.324032      38.17
 H      -4.022551     0.484441    -1.474109      20.80
 C      -2.369405     1.717316    -0.905107       1.06
 O      -3.047142     2.956019    -0.950878     215.68
 C      -4.452486     2.914609    -0.485941      96.05
 H      -4.574156     2.665330     0.527531      24.99
 H      -4.565980     4.241165    -0.418904      22.24
 H      -4.829874     2.483595    -1.451151      21.29
 C      -1.111586     1.637610    -0.346361       7.87
 O      -0.550738     2.797192     0.229298     195.82
 C      -0.597168     0.279583    -0.262325      32.85
 H       0.437311     0.248821     0.275508      18.74
 C      -2.405017    -0.945014    -1.377655      22.87
 C      -3.185854    -2.150555    -1.456634      91.75
 H      -4.090143    -2.062654    -2.161303      23.33
 O      -2.339491    -3.200852    -1.786423     234.39
 H      -2.936326    -4.001083    -1.694273      19.35
 C      -3.937573    -2.637820    -0.144785      80.99
 H      -3.129987    -2.928055     0.508952      25.89
 O      -4.721948    -1.524289     0.458313     253.86
 H      -5.143419    -1.854467     1.467967      24.49
 C      -4.949013    -3.785904    -0.576271      95.91
 O      -4.353024    -5.078726    -1.029663     316.45
 H      -3.501224    -5.526219    -0.645800      25.56
 H      -5.528094    -3.418159    -1.391787      28.69
 H      -5.591583    -3.778035     0.105550      32.54
55
name = lig-etoh-frame_764
 C       2.284541     1.920539    -1.908972      28.56
 H       1.731330     2.685360    -2.404452      17.93
 C       3.049536     1.545871     0.177429      85.33
 H       2.740818     1.392997     1.243352      20.68
 C       3.504854     0.286687    -0.237391      39.13
 O       4.234723    -0.658287     0.571284     235.93
 C       4.098341    -0.439986     2.040001     106.68
 H       2.969160    -0.493309     2.354059      25.69
 H       4.573255     0.493434     2.385635      26.42
 H       4.643070    -1.273795     2.589271      25.73
 C       3.256784    -0.228643    -1.489412      28.49
 O       3.817323    -1.405525    -1.978983     222.64
 H       4.358751    -1.824608    -1.286394      27.03
 C       2.610534     0.569542    -2.356448      71.80
 H       2.191030     0.377589    -3.441675      24.69
 C       2.405199     2.337053    -0.664252      81.40
 C       1.741465     3.635802    -0.314920     125.45
 H       2.134811     4.731971    -0.891481      20.13
 O       1.890590     3.943214     1.019942     273.25
 H       2.767778     4.434282     1.155640      28.89
 C       0.163833     3.721590    -0.538014      72.09
 H       0.099742     3.721777    -1.589638      20.11
 C      -0.473329     5.192536     0.031078      89.86
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 O       0.071609     6.245424    -0.782682     272.41
 H       0.069309     5.744768    -1.718746      25.86
 H      -0.103035     5.162974     1.101381      22.43
 H      -1.592892     5.137617     0.053242      23.87
 C      -1.182695    -0.950411    -0.688595      23.57
 H      -0.873744    -1.956283    -0.833740      18.83
 C      -3.012769     0.400983    -1.285495      43.76
 H      -4.056872     0.559291    -1.637597      18.58
 C      -2.426091     1.637636    -0.963585      -4.07
 O      -3.027095     2.981080    -0.895009     191.95
 C      -4.404360     2.956060    -0.543176     110.66
 H      -4.681062     2.227878     0.412445      22.91
 H      -4.482457     3.936242    -0.815074      25.68
 H      -4.927933     2.403102    -1.454386      23.47
 C      -1.090384     1.601410    -0.318718      -5.70
 O      -0.542130     2.788035     0.263388     190.58
 C      -0.450412     0.325741    -0.279193      38.53
 H       0.373071     0.137861     0.349524      20.01
 C      -2.368929    -0.944881    -1.367483      27.83
 C      -3.246281    -2.182386    -1.451147      94.04
 H      -3.931145    -2.177788    -2.287634      23.51
 O      -2.343503    -3.215775    -1.775063     236.36
 H      -2.839317    -4.051941    -1.678349      20.71
 C      -3.861954    -2.659788    -0.130862      67.23
 H      -3.090233    -3.200264     0.625391      21.35
 O      -4.754356    -1.534327     0.480098     266.76
 H      -4.764518    -1.939457     1.302593      26.20
 C      -4.918419    -3.805759    -0.628476      57.84
 O      -4.328555    -5.021339    -1.021280     277.02
 H      -3.647716    -5.265538    -0.359984      29.45
 H      -5.559224    -3.479981    -1.505767      26.59
 H      -5.626016    -3.653202     0.571294      24.41
55
name = lig-etoh-frame_765
 C       2.248746     1.931031    -1.923208      55.41
 H       1.666165     2.532615    -2.728298      18.91
 C       3.040435     1.421811     0.221939     102.77
 H       2.771261     1.676250     1.239565      22.30
 C       3.499227     0.213455    -0.248515      28.42
 O       4.201799    -0.672342     0.535888     220.97
 C       4.075616    -0.454709     2.050718     100.13
 H       3.030947    -0.212038     2.092032      26.53
 H       4.533934     0.508567     2.353573      26.02
 H       4.683982    -1.277369     2.410293      25.36
 C       3.250066    -0.238923    -1.518633      19.24
 O       3.789871    -1.409841    -1.937665     176.86
 H       4.449805    -1.695861    -1.285792      25.79
 C       2.612300     0.593174    -2.363615      74.24
 H       2.515520     0.403727    -3.376736      29.59
 C       2.430235     2.410177    -0.661034     106.38
 C       1.747075     3.685902    -0.305331     134.68
 H       2.045588     4.613961    -0.741692      23.67
 O       1.930999     3.954106     1.030608     316.75
 H       2.839461     4.127020     1.160049      33.83
 C       0.116062     3.708106    -0.516737      62.90
 H      -0.129918     3.632573    -1.649129      21.41
 C      -0.418863     5.167745     0.000454     105.60
 O       0.073853     6.264376    -0.716169     286.73
 H       0.247432     5.970636    -1.643735      29.91
 H      -0.171034     5.299738     1.060955      24.50
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 H      -1.477822     4.866759    -0.065895      24.46
 C      -1.147616    -0.898448    -0.703442      13.84
 H      -0.652259    -1.927806    -0.474924      18.58
 C      -3.108975     0.408882    -1.291619      64.35
 H      -4.067770     0.452300    -1.810321      18.81
 C      -2.436195     1.576140    -0.967186       3.16
 O      -2.967808     2.943116    -0.840236     204.97
 C      -4.366877     2.939722    -0.644817     115.02
 H      -4.683497     2.348164     0.145900      27.02
 H      -4.960213     4.100104    -0.857161      23.44
 H      -5.162899     2.370881    -1.269934      24.45
 C      -1.075047     1.543989    -0.317126      -6.87
 O      -0.545600     2.732047     0.298085     177.50
 C      -0.357071     0.326961    -0.292371      13.09
 H       0.566030     0.096108     0.457261      17.87
 C      -2.404243    -0.827940    -1.301616      29.08
 C      -3.275347    -2.197404    -1.449584      75.32
 H      -3.969759    -2.056029    -2.328701      23.15
 O      -2.310512    -3.261869    -1.783871     174.12
 H      -2.751984    -4.307299    -1.736095      16.03
 C      -3.863728    -2.667757    -0.143264      95.50
 H      -3.220577    -3.120687     0.545579      24.24
 O      -4.741319    -1.587205     0.488196     302.77
 H      -4.586236    -1.879565     1.501371      24.37
 C      -4.916461    -3.764653    -0.581296     106.60
 O      -4.298372    -4.981124    -1.003064     288.29
 H      -3.819159    -5.140829    -0.154166      30.32
 H      -5.541109    -3.479214    -1.397576      28.23
 H      -5.453196    -4.013888     0.208346      30.97
55
name = lig-etoh-frame_766
 C       2.190449     1.918179    -2.033701      94.09
 H       1.794704     2.348658    -2.893332      24.09
 C       2.991752     1.371161     0.281108      89.40
 H       3.152318     1.860537     1.273433      22.17
 C       3.501869     0.148299    -0.201745      18.81
 O       4.183863    -0.698066     0.538231     227.56
 C       4.069583    -0.434342     1.998352      90.48
 H       2.967661    -0.275542     2.209535      24.64
 H       4.635117     0.495480     2.265351      23.72
 H       4.494512    -1.461678     2.432787      23.33
 C       3.272709    -0.261870    -1.558941      13.19
 O       3.752044    -1.441295    -1.913090     110.01
 H       4.718859    -1.580231    -1.315516      20.66
 C       2.589609     0.690009    -2.405318      51.52
 H       2.735464     0.313510    -3.508076      22.37
 C       2.457934     2.438689    -0.667437      77.53
 C       1.702669     3.728874    -0.295425     106.01
 H       2.161425     4.597066    -1.147767      20.74
 O       1.980838     3.979892     1.096565     283.99
 H       2.989587     3.867494     1.255588      27.30
 C       0.114832     3.739412    -0.506126      69.89
 H      -0.342487     3.480984    -1.450138      23.18
 C      -0.377550     5.070764    -0.022881      99.08
 O       0.082470     6.299137    -0.657287     229.04
 H       0.269776     6.283816    -1.648081      28.94
 H      -0.195218     5.402660     1.020380      23.46
 H      -1.477991     4.956335    -0.242597      24.27
 C      -1.051651    -0.828666    -0.704628      33.96
 H      -0.554432    -1.633679    -0.205825      22.18
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 C      -3.200438     0.423684    -1.339717      56.24
 H      -4.149719     0.369240    -1.866165      17.60
 C      -2.395048     1.570862    -0.900198       4.69
 O      -2.911580     2.866954    -0.809998     178.77
 C      -4.418954     2.955755    -0.767049     102.56
 H      -4.632141     2.618253     0.434280      23.81
 H      -4.906416     3.831642    -0.572823      27.35
 H      -5.004561     2.333285    -1.545221      24.79
 C      -1.065564     1.488305    -0.337764       4.56
 O      -0.560256     2.648461     0.331494     168.84
 C      -0.323283     0.278926    -0.282736      27.79
 H       0.554584     0.264839     0.204700      20.64
 C      -2.465798    -0.749553    -1.200434      -9.31
 C      -3.225645    -2.180530    -1.463370      71.64
 H      -4.052473    -1.933289    -2.154809      24.12
 O      -2.266530    -3.327938    -1.809943     215.05
 H      -2.728532    -4.080859    -1.728234      21.96
 C      -3.971546    -2.651065    -0.176030      85.01
 H      -3.066824    -2.984474     0.577881      19.22
 O      -4.696266    -1.674693     0.512415     325.08
 H      -4.581676    -1.523994     1.563602      27.09
 C      -4.913545    -3.706476    -0.531020      91.34
 O      -4.254065    -4.957627    -0.983631     237.99
 H      -3.814616    -5.403058    -0.175078      27.22
 H      -5.613582    -3.284873    -1.308675      25.99
 H      -5.721806    -4.412419     0.261691      22.45
55
name = lig-etoh-frame_767
 C       2.145953     1.944431    -2.104611      77.55
 H       1.804062     2.629921    -2.994727      23.40
 C       2.925976     1.429647     0.302795      97.48
 H       3.589311     1.726178     1.168418      26.52
 C       3.459805     0.140629    -0.188302      12.14
 O       4.189685    -0.754684     0.586167     225.97
 C       4.068318    -0.440616     1.939549     125.86
 H       3.073574    -0.416243     2.405261      26.44
 H       4.752810     0.352907     2.230613      26.16
 H       4.261145    -1.316381     2.486395      26.72
 C       3.272053    -0.206037    -1.557809       8.30
 O       3.753416    -1.506671    -1.903978     207.54
 H       4.593420    -1.599201    -1.639450      29.26
 C       2.633763     0.678939    -2.478942      26.65
 H       2.667682     0.397085    -3.523792      20.67
 C       2.443711     2.377174    -0.717660      62.64
 C       1.693453     3.745351    -0.317503     111.75
 H       2.078613     4.420449    -1.113899      23.69
 O       2.036149     4.028879     1.156261     294.34
 H       2.977854     3.701063     1.279485      27.30
 C       0.150288     3.732085    -0.473777      68.65
 H      -0.225590     3.496529    -1.485672      21.82
 C      -0.401625     5.016716    -0.049167      98.11
 O       0.109817     6.348426    -0.602627     193.63
 H       0.065748     6.329027    -1.667932      26.55
 H      -0.245106     5.190927     1.048924      24.44
 H      -1.448947     5.174029    -0.247726      24.69
 C      -1.001841    -0.780440    -0.694690      50.09
 H      -0.634948    -1.758253    -0.264286      22.74
 C      -3.213056     0.450345    -1.379123      41.90
 H      -4.249079     0.453865    -1.790481      23.22
 C      -2.381695     1.572308    -0.815683       2.09
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 O      -2.889507     2.810368    -0.799782     160.93
 C      -4.469662     2.911958    -0.803972      86.87
 H      -4.590977     2.670581     0.162976      26.37
 H      -4.629353     4.197447    -0.563072      22.68
 H      -4.645395     2.367444    -1.807809      22.83
 C      -1.055641     1.465568    -0.358794      23.20
 O      -0.566581     2.570349     0.368712     124.20
 C      -0.352409     0.281188    -0.283845      50.99
 H       0.814444     0.392542     0.018052      20.21
 C      -2.482918    -0.772227    -1.093439     -16.18
 C      -3.140359    -2.133665    -1.456070      63.40
 H      -3.966565    -1.967065    -2.197504      22.63
 O      -2.225457    -3.331718    -1.845840     134.19
 H      -2.995536    -4.188564    -1.625437      10.89
 C      -4.008026    -2.636484    -0.131909     110.75
 H      -3.186455    -2.949858     0.376462      23.97
 O      -4.679156    -1.706364     0.543361     417.86
 H      -4.468029    -1.596500     1.390457      34.13
 C      -4.990605    -3.757914    -0.458654      91.92
 O      -4.211200    -4.936819    -0.990251     302.49
 H      -3.751472    -5.539628    -0.399720      29.76
 H      -5.602035    -3.275409    -1.231918      27.38
 H      -5.633707    -3.946253     0.247050      28.98
55
name = lig-etoh-frame_768
 C       2.142250     1.980473    -2.142398      66.05
 H       1.833711     2.817130    -2.702326      22.74
 C       2.922912     1.483934     0.262930     105.57
 H       3.577203     1.728625     1.063398      27.06
 C       3.388285     0.184361    -0.199648       7.65
 O       4.176295    -0.806709     0.614090     193.10
 C       4.076253    -0.473517     1.947885     104.49
 H       3.046281    -0.184898     2.334138      25.43
 H       4.840945     0.302514     2.296581      24.89
 H       4.428561    -1.426529     2.616130      23.98
 C       3.278385    -0.165226    -1.539757      14.82
 O       3.727545    -1.555514    -1.923366     158.02
 H       4.810407    -1.703404    -1.792563      21.75
 C       2.697284     0.645460    -2.549908      22.87
 H       2.532460     0.403180    -3.633986      22.05
 C       2.361047     2.304796    -0.777067      50.28
 C       1.724947     3.685118    -0.294394     111.53
 H       2.085050     4.659100    -1.038065      20.28
 O       2.085711     4.087383     1.163598     323.91
 H       2.914082     3.690450     1.273495      28.91
 C       0.187598     3.665211    -0.455113      65.14
 H       0.129824     3.549219    -1.581481      19.47
 C      -0.464863     5.056846    -0.038481      94.32
 O       0.143383     6.381110    -0.562612     222.29
 H      -0.081164     6.198096    -1.460952      30.46
 H      -0.302850     4.943683     1.035512      24.18
 H      -1.573286     5.114011    -0.223624      24.00
 C      -1.060830    -0.850309    -0.679291      36.60
 H      -0.743882    -1.924578    -0.691367      21.53
 C      -3.121702     0.453284    -1.359262      57.87
 H      -4.159481     0.579301    -1.608630      24.88
 C      -2.430390     1.538040    -0.768511       2.58
 O      -2.902551     2.804686    -0.790951     167.13
 C      -4.420986     2.940764    -0.841480     100.48
 H      -4.917952     2.211983     0.135251      22.57
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 H      -4.395120     3.965434    -1.036922      25.84
 H      -4.741089     2.547069    -1.791946      26.58
 C      -1.053980     1.495046    -0.355457      20.87
 O      -0.546309     2.531899     0.398592     136.74
 C      -0.323034     0.350338    -0.280080      58.74
 H       0.681581     0.322363    -0.146876      22.88
 C      -2.452969    -0.819574    -1.030820       6.35
 C      -3.079012    -2.100756    -1.428080      72.41
 H      -3.665113    -2.011898    -2.365666      21.01
 O      -2.234947    -3.314859    -1.864294     218.33
 H      -2.831291    -3.984509    -1.630439      20.06
 C      -3.971920    -2.662476    -0.111714      71.96
 H      -3.067579    -3.237422     0.522838      18.37
 O      -4.709082    -1.670357     0.574006     300.54
 H      -4.261850    -1.792079     1.577233      21.21
 C      -5.027834    -3.817816    -0.425851      45.04
 O      -4.205940    -4.907023    -1.027557     265.24
 H      -3.614604    -5.479734    -0.439348      26.85
 H      -5.630821    -3.547712    -1.326415      26.13
 H      -5.730603    -3.648275     0.716964      22.86
55
name = lig-etoh-frame_769
 C       2.198612     1.954332    -2.140138      58.95
 H       1.784150     2.854723    -2.704467      17.81
 C       2.967460     1.486834     0.165295      60.75
 H       3.257904     2.023003     1.167860      18.09
 C       3.348024     0.219559    -0.190830      29.09
 O       4.122838    -0.821112     0.592684     192.71
 C       4.111157    -0.520940     2.054799     117.81
 H       3.147612     0.000783     2.147266      25.16
 H       4.797950     0.290844     2.274189      27.06
 H       4.456865    -1.368499     2.485502      27.24
 C       3.300324    -0.198489    -1.577057      33.95
 O       3.700915    -1.566479    -1.942834     148.10
 H       4.750455    -1.708844    -1.887096      22.09
 C       2.731461     0.675233    -2.602430      43.87
 H       2.498915     0.244484    -3.647594      21.17
 C       2.255905     2.280959    -0.791754      68.60
 C       1.776120     3.640000    -0.235508     111.08
 H       2.067900     4.578148    -0.809998      22.85
 O       2.120284     4.135873     1.116555     298.44
 H       3.034180     3.742056     1.350241      27.55
 C       0.221588     3.616082    -0.456539      63.65
 H       0.202734     3.424748    -1.507811      20.34
 C      -0.525406     5.106408    -0.000913      88.96
 O       0.156836     6.363706    -0.509766     195.96
 H      -0.065621     6.225039    -1.550968      25.54
 H      -0.397654     5.010961     1.126034      23.21
 H      -1.566598     4.932669    -0.254619      23.62
 C      -1.131358    -0.933559    -0.655763      45.76
 H      -0.633537    -1.855853    -0.989818      21.93
 C      -2.991420     0.416857    -1.275028      76.88
 H      -4.069227     0.555028    -1.504725      25.99
 C      -2.461919     1.511208    -0.749652      12.83
 O      -2.954521     2.819212    -0.775758     230.31
 C      -4.330754     2.917785    -0.853119     132.50
 H      -5.066923     2.406352    -0.416029      27.12
 H      -4.491347     4.114892    -1.271317      23.06
 H      -4.980104     2.565245    -1.852261      24.61
 C      -1.069132     1.531755    -0.317498      11.27
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 O      -0.493496     2.561226     0.403728     174.50
 C      -0.339679     0.331561    -0.322866      27.24
 H       0.795559     0.251057    -0.103369      19.99
 C      -2.392019    -0.842805    -1.022195      30.77
 C      -3.066862    -2.127796    -1.396354      86.98
 H      -3.552810    -1.883568    -2.355412      20.65
 O      -2.230805    -3.248560    -1.867250     189.57
 H      -2.847332    -4.129030    -1.644688      14.78
 C      -3.910564    -2.729890    -0.126537      89.99
 H      -3.306538    -3.204268     0.543519      22.12
 O      -4.713074    -1.620191     0.639273     329.56
 H      -4.441509    -1.861434     1.606546      24.84
 C      -5.033116    -3.824879    -0.379324      96.87
 O      -4.230082    -4.900471    -1.057120     267.18
 H      -3.509181    -5.227467    -0.409482      27.62
 H      -5.760260    -3.790987    -1.201959      26.05
 H      -5.460915    -3.949298     0.482711      31.34
55
name = lig-etoh-frame_770
 C       2.259304     1.923335    -2.146977      62.81
 H       1.793107     2.508020    -2.953912      21.68
 C       3.008046     1.514291     0.093415      66.64
 H       2.816898     1.964096     1.023742      20.39
 C       3.384749     0.172221    -0.200430      20.44
 O       4.042679    -0.792720     0.560926     190.46
 C       4.147400    -0.518268     2.112531      88.79
 H       3.122559    -0.113186     2.345673      25.65
 H       4.925331     0.307924     2.247406      25.37
 H       4.344145    -1.619362     2.602372      23.87
 C       3.312820    -0.247565    -1.650696      13.41
 O       3.667694    -1.541242    -1.964882     202.79
 H       4.564634    -1.676607    -1.822510      27.02
 C       2.753444     0.697628    -2.608696      41.81
 H       2.625384     0.252512    -3.551185      23.63
 C       2.206494     2.282257    -0.755244      79.69
 C       1.790816     3.615280    -0.170946     102.50
 H       2.180229     4.502741    -0.986673      20.34
 O       2.154977     4.152555     1.061881     308.65
 H       3.101911     4.020264     1.398440      29.10
 C       0.244766     3.626587    -0.421182      59.05
 H      -0.036303     3.268122    -1.489553      20.56
 C      -0.535054     5.109596     0.041724      90.06
 O       0.127894     6.299232    -0.476799     222.80
 H       0.208141     6.406327    -1.436865      29.69
 H      -0.516167     5.307844     1.098394      24.97
 H      -1.575537     4.937372    -0.358325      24.19
 C      -1.065369    -0.962630    -0.616623      56.90
 H      -0.371769    -1.773343    -0.994372      21.10
 C      -2.943263     0.344659    -1.175516      59.80
 H      -3.958479     0.324250    -1.538805      23.62
 C      -2.397310     1.565085    -0.712115      17.70
 O      -3.006840     2.812809    -0.752190     226.11
 C      -4.322607     2.970991    -0.990478     127.77
 H      -5.213333     2.575858    -0.155386      24.32
 H      -4.627136     3.941875    -0.906463      27.35
 H      -4.630638     2.493727    -1.977277      25.73
 C      -1.071492     1.517250    -0.250477       8.18
 O      -0.423803     2.634546     0.387494     187.42
 C      -0.398119     0.242401    -0.386950      20.60
 H       0.646492     0.236264     0.001503      20.02
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 C      -2.372077    -0.883473    -1.050669      28.06
 C      -3.104668    -2.187984    -1.371428      94.38
 H      -3.845544    -1.769958    -2.134274      21.70
 O      -2.221605    -3.182811    -1.849876     214.05
 H      -2.755582    -4.103774    -1.866530      17.95
 C      -3.938647    -2.739816    -0.160965      85.55
 H      -3.207753    -3.178080     0.714297      17.79
 O      -4.686769    -1.594845     0.696143     309.49
 H      -4.685867    -1.791027     1.637619      27.96
 C      -4.975804    -3.816986    -0.407298      80.76
 O      -4.250506    -4.920776    -1.066813     281.95
 H      -3.514659    -5.104168    -0.486112      28.42
 H      -5.959665    -3.611502    -0.927975      25.07
 H      -5.377666    -4.572069     0.664843      23.89
55
name = lig-etoh-frame_771
 C       2.284015     1.909771    -2.170476      78.17
 H       1.818305     2.305359    -3.070833      20.74
 C       3.018064     1.507280     0.060666      63.46
 H       2.714747     1.645573     1.181632      19.26
 C       3.448006     0.118277    -0.278983      16.27
 O       3.965935    -0.757250     0.570301     189.06
 C       4.163587    -0.523689     2.120269     111.86
 H       3.230162    -0.298855     2.680304      26.53
 H       4.995584     0.110184     2.292299      27.33
 H       4.237669    -1.435479     2.539176      27.95
 C       3.311776    -0.246095    -1.671537      23.58
 O       3.623024    -1.514108    -2.009557     132.19
 H       4.654605    -1.794253    -1.565279      20.24
 C       2.793963     0.666675    -2.551686      40.15
 H       2.763633     0.408253    -3.735466      23.11
 C       2.237088     2.283229    -0.753885      87.36
 C       1.778730     3.634820    -0.207239     114.18
 H       2.210856     4.309451    -1.143084      22.10
 O       2.183659     4.155995     1.042889     308.50
 H       3.117971     4.301944     1.158227      32.57
 C       0.231151     3.692692    -0.370284      82.88
 H      -0.076302     3.500293    -1.355182      23.09
 C      -0.513054     5.075421     0.033217      99.81
 O       0.096723     6.245760    -0.442431     258.78
 H       0.350511     6.261001    -1.385793      31.18
 H      -0.634681     5.430468     1.127560      23.98
 H      -1.519325     5.058182    -0.371021      25.38
 C      -0.933630    -0.992897    -0.613175      63.27
 H      -0.270446    -1.811991    -0.689841      21.54
 C      -2.965805     0.299707    -1.079397      43.21
 H      -3.951297     0.201091    -1.578644      19.97
 C      -2.323759     1.623910    -0.675737      11.62
 O      -3.009385     2.804936    -0.706669     198.45
 C      -4.445318     2.996908    -1.114776      91.28
 H      -4.748645     2.623015    -0.201523      25.02
 H      -4.651610     4.154420    -0.684299      23.01
 H      -4.283763     2.499134    -2.167554      22.07
 C      -1.040004     1.485883    -0.173981      18.78
 O      -0.368647     2.679150     0.386551     192.72
 C      -0.444411     0.207873    -0.394060      43.66
 H       0.552844     0.198049    -0.014373      20.85
 C      -2.347844    -0.973454    -1.073307       8.52
 C      -3.200467    -2.203301    -1.348264      93.53
 H      -4.106826    -1.975017    -1.940615      23.04
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 O      -2.210046    -3.136404    -1.841878     267.57
 H      -2.686340    -3.910785    -2.030056      24.72
 C      -3.986212    -2.711886    -0.077699      95.93
 H      -3.191748    -3.042893     0.469646      24.85
 O      -4.638891    -1.582343     0.703710     293.96
 H      -4.896758    -1.934699     1.752304      24.83
 C      -4.943064    -3.885384    -0.383603     107.89
 O      -4.273195    -4.946084    -1.104678     340.01
 H      -3.458592    -5.192814    -0.527817      28.23
 H      -5.860381    -3.348779    -0.684184      28.11
 H      -5.130073    -4.373436     0.402897      31.72
55
name = lig-etoh-frame_772
 C       2.286240     1.898059    -2.182417      89.44
 H       1.778876     2.517838    -3.010236      16.88
 C       3.008907     1.411626     0.094914      62.31
 H       2.996831     1.354996     1.146985      20.47
 C       3.480137     0.169944    -0.373795      29.41
 O       3.911229    -0.754228     0.637412     202.77
 C       4.140047    -0.527385     2.081147     102.57
 H       3.351731    -0.154201     2.807464      24.90
 H       5.115046     0.042196     2.335764      25.52
 H       4.433089    -1.683980     2.404613      23.08
 C       3.331941    -0.244062    -1.623935      32.88
 O       3.628424    -1.525564    -2.062255     232.66
 H       4.277308    -1.872781    -1.517851      27.86
 C       2.827670     0.644336    -2.547750      39.65
 H       2.890650     0.553314    -3.531233      28.79
 C       2.312471     2.289507    -0.803222     105.41
 C       1.750702     3.684385    -0.309798     134.20
 H       2.206625     4.294250    -1.214918      27.68
 O       2.207932     4.149032     1.034894     240.99
 H       3.147825     4.552042     0.773797      30.55
 C       0.205236     3.799697    -0.321907      77.96
 H       0.026050     3.824997    -1.492162      18.84
 C      -0.500232     5.042532     0.037930     115.73
 O       0.092759     6.232787    -0.427151     278.52
 H       0.351285     5.893999    -1.396647      29.63
 H      -0.649855     5.100887     1.090764      25.79
 H      -1.551886     4.993491    -0.363148      24.02
 C      -0.893868    -1.074439    -0.667443      32.15
 H      -0.246119    -1.987822    -0.321629      20.38
 C      -2.983491     0.279021    -0.998977      45.22
 H      -3.977184     0.349704    -1.462954      20.32
 C      -2.329503     1.609423    -0.659452      -3.30
 O      -2.967822     2.828321    -0.652181     131.29
 C      -4.505125     3.034198    -1.182610      93.35
 H      -4.880391     2.153433    -0.405968      21.82
 H      -4.562269     4.041000    -1.169321      27.14
 H      -4.610397     2.732902    -2.178059      27.59
 C      -0.998466     1.497026    -0.118717      24.18
 O      -0.339218     2.660567     0.422344     170.28
 C      -0.402545     0.261330    -0.319017      26.61
 H       0.759072     0.197586    -0.055300      20.27
 C      -2.308969    -1.032169    -1.063629       2.07
 C      -3.306807    -2.176185    -1.311658      73.94
 H      -4.111099    -2.174547    -2.121502      22.01
 O      -2.213502    -3.101574    -1.830425     160.17
 H      -2.774905    -3.984230    -2.293564      18.51
 C      -4.004082    -2.670159     0.047857      68.06
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 H      -2.989302    -3.100911     0.577513      21.61
 O      -4.597296    -1.597786     0.703603     363.76
 H      -4.821583    -2.025947     1.465731      28.12
 C      -4.896476    -3.913358    -0.347580      65.36
 O      -4.290162    -4.973581    -1.173115     297.12
 H      -3.530366    -5.359329    -0.651682      28.10
 H      -5.774862    -3.418876    -0.834031      26.91
 H      -5.211995    -4.279343     0.947709      24.20
55
name = lig-etoh-frame_773
 C       2.280275     1.901760    -2.175808      37.18
 H       1.886429     2.669583    -2.770349      23.99
 C       2.974725     1.327445     0.112986      79.91
 H       3.228486     1.477836     1.212247      23.63
 C       3.519477     0.239099    -0.339058      38.86
 O       3.862126    -0.765384     0.697277     244.35
 C       4.158976    -0.569483     2.053984     128.91
 H       3.397583    -0.040439     2.624356      26.09
 H       5.035483     0.027116     2.185031      27.24
 H       4.459661    -1.524058     2.221510      26.17
 C       3.363212    -0.284941    -1.637238      23.13
 O       3.633204    -1.544308    -2.123100     189.26
 H       4.173593    -2.042805    -1.386383      24.44
 C       2.838177     0.674975    -2.557682      49.12
 H       3.008168     0.400484    -3.745276      20.01
 C       2.396627     2.298972    -0.828021      58.15
 C       1.731833     3.727637    -0.390866      92.68
 H       2.168794     4.604617    -1.244878      20.45
 O       2.252988     4.138887     0.987798     248.58
 H       3.018769     4.696760     0.707254      27.13
 C       0.204712     3.854287    -0.366541      72.13
 H       0.041540     3.793072    -1.402075      20.13
 C      -0.545074     5.030397     0.094588     114.20
 O       0.110639     6.220777    -0.443810     274.98
 H       0.267630     5.970479    -1.345488      32.26
 H      -0.569376     4.853409     1.229795      22.74
 H      -1.532696     4.833548    -0.327669      23.71
 C      -0.912263    -1.108040    -0.708105      31.37
 H      -0.476906    -1.933695    -0.279384      24.03
 C      -2.958999     0.296299    -0.940337      53.43
 H      -3.993236     0.458616    -1.249642      21.92
 C      -2.375358     1.526972    -0.637939      -1.95
 O      -2.937847     2.864667    -0.620662      96.91
 C      -4.492146     2.977532    -1.190566      94.30
 H      -5.293297     2.325897    -0.921016      25.09
 H      -4.641501     4.181836    -1.374278      23.35
 H      -4.931720     2.785488    -2.345717      24.17
 C      -0.980563     1.539773    -0.107452       5.62
 O      -0.320663     2.621450     0.465746     117.84
 C      -0.281162     0.265653    -0.214037      10.34
 H       0.704884     0.293035    -0.052987      22.78
 C      -2.303216    -1.009935    -1.025302       3.97
 C      -3.348928    -2.162015    -1.281790      84.30
 H      -3.920528    -2.044099    -2.182232      22.93
 O      -2.261349    -3.115045    -1.827481     268.47
 H      -2.669697    -3.805727    -2.288199      23.67
 C      -3.915106    -2.678914     0.109200      89.81
 H      -3.173150    -3.045512     0.734201      24.41
 O      -4.570602    -1.618320     0.691713     324.15
 H      -4.851325    -2.012888     1.674446      24.57
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 C      -4.869611    -3.925602    -0.226527     103.93
 O      -4.315419    -4.989259    -1.225095     284.62
 H      -3.605709    -5.474348    -0.779838      28.95
 H      -5.686048    -3.777667    -0.975819      26.68
 H      -5.271777    -4.198207     0.624501      32.18
55
name = lig-etoh-frame_774
 C       2.296358     1.916641    -2.138950      54.40
 H       1.973424     2.784519    -2.858129      24.68
 C       2.914297     1.389970     0.149491      87.79
 H       3.224183     1.885012     1.080286      23.93
 C       3.579636     0.169774    -0.253702      19.64
 O       3.813023    -0.788023     0.686286     232.68
 C       4.203849    -0.572762     2.022382      97.19
 H       3.281810    -0.106266     2.543188      23.76
 H       5.098428     0.156894     2.034624      23.92
 H       4.420677    -1.679812     2.484874      22.83
 C       3.380358    -0.288422    -1.691191       3.97
 O       3.655879    -1.564427    -2.169787     166.07
 H       4.005891    -2.181721    -1.315786      22.43
 C       2.861559     0.680569    -2.621847      51.11
 H       2.896751     0.310073    -3.555948      23.06
 C       2.452202     2.323146    -0.810881      49.66
 C       1.773673     3.772239    -0.435268     108.18
 H       1.959609     4.698925    -0.996999      20.56
 O       2.291315     4.127577     0.906318     286.76
 H       3.014900     4.739123     0.870574      29.75
 C       0.228475     3.810281    -0.446922      48.21
 H      -0.191581     3.486850    -1.504439      19.46
 C      -0.589678     5.019061     0.174724      98.40
 O       0.116791     6.211254    -0.445930     216.41
 H       0.145347     6.200155    -1.486327      26.77
 H      -0.465729     5.079245     1.241512      23.96
 H      -1.622771     4.870884    -0.192084      23.37
 C      -0.954979    -1.018820    -0.697874      24.14
 H      -0.565295    -2.098509    -0.430348      21.92
 C      -2.941686     0.324819    -0.913330      52.48
 H      -4.047746     0.341833    -1.044421      22.42
 C      -2.365723     1.489174    -0.574782       3.87
 O      -2.971958     2.862985    -0.626156     107.66
 C      -4.470378     2.956141    -1.261019     109.30
 H      -5.549003     2.630975    -0.820300      25.20
 H      -4.692977     3.943439    -1.032304      26.84
 H      -4.454014     2.649412    -2.270127      27.39
 C      -0.967503     1.520134    -0.135637      -2.40
 O      -0.304378     2.599321     0.493830     109.31
 C      -0.231073     0.232736    -0.140282       3.32
 H       0.958185     0.333200     0.117718      18.04
 C      -2.336646    -0.933230    -0.968203      15.60
 C      -3.258701    -2.164781    -1.247610      80.40
 H      -4.008610    -1.722765    -2.030259      21.64
 O      -2.317636    -3.135629    -1.815092     256.33
 H      -2.818152    -3.885264    -2.279389      19.55
 C      -3.839395    -2.733448     0.084245      86.91
 H      -3.035093    -3.072387     0.900324      20.11
 O      -4.581312    -1.638388     0.711085     348.16
 H      -4.724670    -1.677954     1.746730      27.99
 C      -4.834971    -3.925598    -0.192543      87.15
 O      -4.336006    -5.000576    -1.239959     224.12
 H      -3.576762    -5.581321    -0.840890      26.19
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 H      -5.692789    -3.709909    -0.859840      26.47
 H      -5.518607    -4.580477     0.770621      24.80
55
name = lig-etoh-frame_775
 C       2.344421     1.945727    -2.145254      73.18
 H       2.066754     2.556900    -2.926536      27.43
 C       2.907701     1.498313     0.178546      71.32
 H       3.074994     2.109017     1.075866      22.33
 C       3.572454     0.105254    -0.218260      14.77
 O       3.785603    -0.857398     0.643753     227.26
 C       4.246068    -0.566559     2.015003     117.97
 H       3.393144    -0.208601     2.541443      26.23
 H       5.045700     0.121978     2.028334      27.07
 H       4.365631    -1.395621     2.636971      26.55
 C       3.395699    -0.247937    -1.697445      13.45
 O       3.684887    -1.585124    -2.189687     235.31
 H       3.849428    -2.078882    -1.497139      30.78
 C       2.880799     0.676267    -2.629637      39.25
 H       2.667905     0.282396    -3.760709      20.63
 C       2.458420     2.377512    -0.806707      36.05
 C       1.837379     3.791126    -0.425812      92.09
 H       2.053433     4.807522    -1.209576      17.85
 O       2.308133     4.111016     0.833122     274.89
 H       3.122773     4.740443     0.956880      26.51
 C       0.206871     3.696270    -0.498937      55.25
 H      -0.273931     3.375109    -1.377709      21.17
 C      -0.573692     5.008860     0.180961      84.79
 O       0.108438     6.210502    -0.444534     181.98
 H      -0.163835     6.292743    -1.430712      28.02
 H      -0.359579     5.347296     1.244307      22.14
 H      -1.692046     5.033694     0.065700      23.49
 C      -0.964401    -0.898269    -0.615241      52.45
 H      -0.592676    -1.886038    -0.828473      23.85
 C      -2.995749     0.341306    -0.904188      58.52
 H      -4.060533     0.246158    -0.916801      22.41
 C      -2.307010     1.557354    -0.490323      -5.42
 O      -3.048440     2.810768    -0.639177     169.55
 C      -4.448567     2.937839    -1.294296      76.90
 H      -5.154928     2.563228    -0.598382      25.21
 H      -4.553315     4.084693    -0.936112      22.81
 H      -3.871509     2.540166    -2.285061      20.34
 C      -0.926552     1.442832    -0.154847       9.41
 O      -0.291257     2.586610     0.495112     147.52
 C      -0.231653     0.194687    -0.108236      55.84
 H       0.711922     0.187496     0.238768      20.87
 C      -2.353537    -0.862605    -0.902563      18.23
 C      -3.120657    -2.143024    -1.213275      95.72
 H      -4.033252    -1.751068    -1.635534      23.11
 O      -2.374950    -3.163625    -1.820512     230.87
 H      -3.140897    -3.966811    -2.066000      15.58
 C      -3.797224    -2.800719     0.098137      97.33
 H      -2.935545    -3.060523     0.674103      23.18
 O      -4.600756    -1.647081     0.722344     399.88
 H      -4.486750    -1.714258     1.648245      30.56
 C      -4.843401    -3.985912    -0.185231      95.95
 O      -4.346587    -5.010428    -1.227668     296.65
 H      -3.620284    -5.493061    -0.802464      30.14
 H      -5.682489    -3.311036    -0.591293      28.21
 H      -5.141127    -4.518779     0.566624      30.02
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name = lig-etoh-frame_776
 C       2.430143     1.938842    -2.188816      39.85
 H       1.984507     2.554965    -3.082727      20.20
 C       2.970276     1.561395     0.184208      81.45
 H       2.944115     1.969462     1.250584      16.74
 C       3.475347     0.161096    -0.260025      60.03
 O       3.791791    -0.975585     0.628096     211.65
 C       4.250155    -0.541040     2.003724      92.24
 H       3.394383     0.017244     2.579217      23.67
 H       5.145486     0.180499     2.023385      25.77
 H       4.557939    -1.514645     2.605809      24.19
 C       3.421254    -0.226526    -1.654031      36.26
 O       3.705750    -1.553003    -2.207181     166.91
 H       3.864423    -2.192791    -1.337533      22.98
 C       2.873632     0.679784    -2.617342      34.87
 H       2.532459     0.463144    -3.589992      21.86
 C       2.438027     2.439914    -0.844271      59.07
 C       1.889610     3.813938    -0.465398     121.50
 H       2.178674     4.367437    -1.345331      24.51
 O       2.316125     4.112101     0.811782     297.85
 H       3.179131     4.587529     0.770979      30.89
 C       0.157883     3.593600    -0.441885      57.39
 H      -0.224262     3.403621    -1.532215      19.13
 C      -0.502575     5.025103     0.148172      96.78
 O       0.070837     6.216792    -0.453910     257.62
 H      -0.308924     6.235567    -1.299314      31.54
 H      -0.200430     5.176856     1.205105      24.46
 H      -1.591385     5.062444     0.190432      24.72
 C      -0.975310    -0.826757    -0.539538      68.34
 H      -0.385945    -1.665077    -1.006973      22.10
 C      -3.059876     0.398323    -0.866193      61.52
 H      -4.180756     0.361723    -0.909079      22.02
 C      -2.309657     1.618846    -0.454920      -8.16
 O      -3.079854     2.748432    -0.610364     207.14
 C      -4.332824     2.935870    -1.282401      90.70
 H      -4.912646     2.110065    -0.665391      21.49
 H      -4.395664     4.005112    -1.420172      24.72
 H      -4.203524     2.623105    -2.271120      27.78
 C      -0.881528     1.413759    -0.127215      15.45
 O      -0.272082     2.568388     0.469900     192.82
 C      -0.286280     0.180189    -0.099904      66.37
 H       0.770222     0.007584     0.381805      18.48
 C      -2.329561    -0.820120    -0.843023      23.20
 C      -3.036062    -2.112606    -1.131092      87.95
 H      -4.051187    -1.917397    -1.659689      20.94
 O      -2.440810    -3.214191    -1.852835     280.62
 H      -3.115151    -3.817180    -1.770398      22.90
 C      -3.765034    -2.829635     0.120512      81.41
 H      -2.825176    -3.170749     0.727717      19.31
 O      -4.608369    -1.684396     0.713592     374.87
 H      -4.229308    -1.911894     1.748590      21.70
 C      -4.821938    -3.995103    -0.242975      66.13
 O      -4.366818    -4.999570    -1.208496     307.40
 H      -3.625606    -5.389200    -0.668219      28.50
 H      -5.650953    -3.286973    -0.356853      27.60
 H      -4.858174    -4.640023     0.930805      24.96
55
name = lig-etoh-frame_777
 C       2.500931     1.963951    -2.250065      31.06
 H       1.964537     2.551611    -2.929722      18.78
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 C       3.046058     1.570572     0.144862      56.21
 H       2.941859     1.629311     1.194193      18.03
 C       3.355291     0.244265    -0.294237      12.52
 O       3.811463    -1.051492     0.626070     177.10
 C       4.246403    -0.517743     2.000692     112.58
 H       3.532677     0.055992     2.481814      27.01
 H       5.110907     0.111905     1.852226      27.69
 H       4.650039    -1.463087     2.334916      25.77
 C       3.432646    -0.225982    -1.623895      10.34
 O       3.718482    -1.485035    -2.177761     184.52
 H       3.977613    -2.161231    -1.393455      20.73
 C       2.860038     0.691928    -2.559046      49.29
 H       2.570695     0.397291    -3.634774      22.67
 C       2.449641     2.444192    -0.881814      71.91
 C       1.879022     3.747716    -0.526583      99.56
 H       2.259049     4.463770    -1.544261      22.21
 O       2.328430     4.144626     0.813740     284.40
 H       3.246002     4.409782     0.685620      32.80
 C       0.121328     3.573091    -0.384085      84.43
 H      -0.020488     3.482508    -1.446460      21.02
 C      -0.394505     5.019192     0.129882     101.17
 O       0.020952     6.222232    -0.465869     259.83
 H      -0.324050     6.209947    -1.463191      27.28
 H      -0.018382     4.852317     1.170556      24.05
 H      -1.526815     4.954383     0.132372      23.56
 C      -1.004079    -0.884875    -0.526939      48.59
 H      -0.219139    -1.600676    -0.870473      21.95
 C      -3.079486     0.461503    -0.787284      41.37
 H      -4.124730     0.534436    -1.000633      19.92
 C      -2.367527     1.585498    -0.480312       7.63
 O      -3.033887     2.737635    -0.545035     241.17
 C      -4.203675     2.872416    -1.264994     129.31
 H      -5.032425     2.205932    -1.028581      25.01
 H      -4.509173     3.948690    -1.555082      24.44
 H      -4.587666     2.494321    -2.476858      23.13
 C      -0.898636     1.483218    -0.067455      21.19
 O      -0.240677     2.545463     0.441557     244.58
 C      -0.274398     0.242569    -0.042447      40.66
 H       0.729085    -0.008224     0.297531      20.13
 C      -2.333591    -0.788762    -0.804962      25.67
 C      -3.062891    -2.112262    -1.057065      96.61
 H      -3.799775    -1.872365    -1.801506      20.61
 O      -2.464432    -3.240507    -1.895701     238.94
 H      -3.197800    -4.043400    -1.579679      13.06
 C      -3.707145    -2.811310     0.131578      92.35
 H      -3.061956    -3.260150     0.925529      19.07
 O      -4.570629    -1.775481     0.736398     384.27
 H      -4.466124    -1.835289     1.673723      29.45
 C      -4.755707    -3.991402    -0.199564     107.09
 O      -4.390928    -4.978160    -1.182969     330.16
 H      -3.609689    -5.422397    -0.661383      27.97
 H      -5.824609    -3.657064    -0.430082      27.44
 H      -4.811009    -4.384662     0.668231      31.40
55
name = lig-etoh-frame_778
 C       2.537234     2.029833    -2.253655      31.80
 H       1.963825     2.673185    -2.996042      18.72
 C       3.092390     1.540756     0.059174      62.35
 H       2.966053     1.560115     1.200916      16.36
 C       3.289904     0.238782    -0.300890       7.79
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 O       3.814520    -1.041204     0.624508     163.77
 C       4.272787    -0.525699     1.925664      97.62
 H       3.431171     0.008612     2.598420      23.58
 H       5.135221     0.153982     1.665994      25.39
 H       4.614491    -1.467899     2.451247      24.81
 C       3.403368    -0.206982    -1.626565      15.04
 O       3.727727    -1.407895    -2.121299     239.31
 H       4.116006    -1.928122    -1.523284      25.96
 C       2.851814     0.673961    -2.539257      50.28
 H       2.857836     0.199513    -3.570820      24.51
 C       2.516373     2.388651    -0.908162      70.16
 C       1.837960     3.683844    -0.582909     110.72
 H       1.974247     4.570392    -1.151535      23.43
 O       2.334455     4.191715     0.794002     259.90
 H       3.395403     4.231802     0.804004      29.56
 C       0.178958     3.656557    -0.399520      74.32
 H      -0.121455     3.386390    -1.459836      19.94
 C      -0.315168     4.949661     0.137664     103.83
 O      -0.029706     6.230928    -0.497534     285.38
 H      -0.072644     6.143350    -1.494398      29.25
 H       0.112243     4.936454     1.190273      22.99
 H      -1.381121     4.828327     0.125780      23.89
 C      -0.973343    -0.923965    -0.511445      27.32
 H      -0.418747    -1.864428    -0.601761      21.36
 C      -3.064864     0.442151    -0.709809      24.37
 H      -4.086466     0.557553    -1.095929      13.74
 C      -2.362992     1.529217    -0.494381      20.48
 O      -2.967314     2.786965    -0.482820     220.81
 C      -4.167808     2.799002    -1.346025     129.06
 H      -5.245471     2.491706    -0.876995      25.10
 H      -4.564823     3.872488    -1.210880      24.71
 H      -4.121930     2.361417    -2.234699      29.69
 C      -0.984677     1.535997    -0.017525      21.02
 O      -0.199968     2.546595     0.447007     198.35
 C      -0.286769     0.302762     0.002395      26.21
 H       0.799449     0.224292     0.233240      18.86
 C      -2.371492    -0.803783    -0.779729      18.32
 C      -3.121258    -2.134763    -1.049379      70.34
 H      -3.860436    -1.679508    -1.797577      19.83
 O      -2.474508    -3.261137    -1.911585     288.46
 H      -2.928275    -4.075318    -1.828501      19.31
 C      -3.708234    -2.777356     0.155247      94.68
 H      -3.082792    -3.224769     0.964824      17.56
 O      -4.534026    -1.865318     0.756264     337.49
 H      -4.675141    -1.871337     1.791648      27.01
 C      -4.714090    -3.937425    -0.165376      94.66
 O      -4.383061    -4.977254    -1.147651     287.55
 H      -3.709468    -5.582188    -0.872772      31.50
 H      -5.734659    -3.932371    -0.594955      25.14
 H      -4.918805    -4.519778     1.030131      25.63
55
name = lig-etoh-frame_779
 C       2.539936     2.060503    -2.270088      29.19
 H       2.166235     2.731254    -3.055372      19.07
 C       3.101390     1.486062     0.025562      58.26
 H       3.042610     1.876092     1.009792      17.28
 C       3.309236     0.116999    -0.279441      18.23
 O       3.791277    -0.959801     0.607894     253.50
 C       4.300957    -0.546786     1.842420     119.44
 H       3.561965    -0.171826     2.464084      27.60
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 H       5.088562     0.208566     1.723191      26.92
 H       4.568632    -1.333583     2.605260      25.50
 C       3.334355    -0.162751    -1.623906      26.08
 O       3.731594    -1.349912    -2.080090     142.72
 H       4.521128    -1.814228    -1.386477      19.26
 C       2.859023     0.678706    -2.583035      56.29
 H       3.019548     0.218132    -3.547214      26.21
 C       2.587206     2.370701    -0.939113      75.52
 C       1.785472     3.650027    -0.531404     113.23
 H       1.849015     4.721313    -1.222281      20.04
 O       2.339330     4.227365     0.758758     315.62
 H       3.271816     4.134037     0.907724      32.55
 C       0.316814     3.707755    -0.498580      69.20
 H      -0.339575     3.411310    -1.350877      19.38
 C      -0.267482     4.903907     0.172370      96.19
 O      -0.064658     6.230551    -0.538279     236.88
 H       0.137472     6.034315    -1.479512      29.66
 H       0.120938     5.222796     1.139065      22.73
 H      -1.385090     4.722637     0.276024      22.42
 C      -0.932331    -0.902481    -0.463499      47.96
 H      -0.771710    -2.032819    -0.261445      19.78
 C      -3.065676     0.322298    -0.677135      41.45
 H      -4.082550     0.411584    -1.065657      15.52
 C      -2.299605     1.575431    -0.449218       7.72
 O      -2.921868     2.838845    -0.444084     185.29
 C      -4.199518     2.779108    -1.351763      82.26
 H      -4.928874     2.472110    -0.658747      25.41
 H      -4.328917     3.906856    -1.265206      23.95
 H      -3.522375     2.191681    -2.338593      19.89
 C      -1.052754     1.519954     0.019265      20.95
 O      -0.161705     2.585227     0.479698      75.84
 C      -0.336518     0.300913     0.006054      34.56
 H       0.778028     0.597730     0.183858      16.73
 C      -2.364046    -0.882608    -0.751355       8.06
 C      -3.186921    -2.154141    -1.124957      68.61
 H      -4.118789    -1.788876    -1.561822      22.35
 O      -2.448067    -3.227938    -1.917487     266.84
 H      -2.960110    -4.116904    -1.936768      15.70
 C      -3.754501    -2.797210     0.195273      85.77
 H      -2.748521    -3.127296     0.738519      19.69
 O      -4.538936    -1.883680     0.785781     309.19
 H      -4.672767    -2.260716     1.835198      21.51
 C      -4.704226    -3.967973    -0.082649     104.63
 O      -4.355492    -4.998098    -1.125008     327.23
 H      -3.697383    -5.740232    -0.883414      29.98
 H      -5.634947    -3.533551    -0.548774      29.09
 H      -4.915138    -4.373148     0.749775      31.96
55
name = lig-etoh-frame_780
 C       2.538654     2.026728    -2.333814      49.70
 H       2.344161     2.788038    -3.083173      19.47
 C       3.085558     1.425913     0.030992      81.98
 H       3.185169     2.096892     0.951965      17.09
 C       3.366046     0.025660    -0.211390       5.29
 O       3.765355    -0.870332     0.557583     234.78
 C       4.335059    -0.547152     1.810806     103.05
 H       3.426462    -0.017006     2.387830      23.72
 H       5.118235     0.243264     1.820661      25.58
 H       4.700366    -1.414578     2.360335      25.82
 C       3.255599    -0.146639    -1.617304      33.20
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 O       3.773611    -1.357444    -2.034963     129.17
 H       4.618306    -1.459736    -1.568294      24.28
 C       2.866124     0.746352    -2.656092      39.76
 H       3.078752     0.397745    -3.771619      23.77
 C       2.621659     2.404936    -0.962903     104.69
 C       1.830476     3.700087    -0.473988     128.36
 H       2.034977     4.256799    -1.376973      24.97
 O       2.309670     4.251111     0.726941     321.99
 H       3.274794     4.095331     0.811242      30.44
 C       0.388122     3.684931    -0.552158      63.47
 H      -0.188851     3.603190    -1.458745      19.47
 C      -0.257868     4.934925     0.205493      88.37
 O      -0.098169     6.214804    -0.584047     224.54
 H       0.259644     5.953847    -1.548412      27.45
 H       0.224360     5.281241     1.202870      21.82
 H      -1.274999     4.656080     0.395051      23.10
 C      -0.947453    -0.910999    -0.384678      70.64
 H      -0.637626    -1.855709    -0.038663      21.75
 C      -3.035496     0.240185    -0.673777      54.79
 H      -4.090740     0.204756    -0.921989      17.49
 C      -2.333465     1.629491    -0.385610      -3.96
 O      -2.890758     2.872254    -0.420147     195.07
 C      -4.137680     2.800720    -1.323754      96.16
 H      -4.812171     2.080248    -0.700806      23.02
 H      -4.151624     3.861472    -1.816858      23.15
 H      -3.785435     2.316073    -2.094857      29.04
 C      -1.006886     1.503580     0.071286      14.89
 O      -0.145981     2.620047     0.514077      82.03
 C      -0.369035     0.284814    -0.007028      52.65
 H       0.605468     0.519854     0.200189      18.97
 C      -2.337612    -0.971188    -0.740550       7.22
 C      -3.250697    -2.192925    -1.191050      68.87
 H      -4.286554    -1.976148    -1.603311      20.40
 O      -2.416251    -3.158564    -1.914273     235.40
 H      -3.180373    -3.940905    -1.913898      15.26
 C      -3.724477    -2.863402     0.181986      81.79
 H      -2.727838    -3.048028     0.602361      20.95
 O      -4.577512    -1.865121     0.842101     324.57
 H      -4.521077    -2.316699     1.860535      19.27
 C      -4.701129    -4.007785    -0.076110      64.09
 O      -4.327851    -5.027709    -1.111327     293.74
 H      -3.690374    -5.627917    -0.589326      27.38
 H      -5.411740    -3.181080    -0.359157      24.99
 H      -5.117157    -4.593674     1.054704      27.74
55
name = lig-etoh-frame_781
 C       2.528639     2.036758    -2.375431      62.64
 H       2.433836     2.863747    -3.159057      23.86
 C       3.053046     1.428316     0.052124      75.24
 H       3.357426     1.838433     1.015356      24.01
 C       3.362409     0.134074    -0.243665      28.52
 O       3.790147    -0.869518     0.543699     223.26
 C       4.338046    -0.502084     1.838716     111.08
 H       3.573487    -0.057460     2.373643      24.68
 H       5.187760     0.226879     1.742242      25.25
 H       4.762188    -1.569122     1.983338      21.96
 C       3.194237    -0.172392    -1.636921      25.11
 O       3.821899    -1.382550    -2.013289     159.00
 H       4.747877    -1.389524    -1.666526      25.52
 C       2.897100     0.773636    -2.737821      32.40
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 H       3.005690     0.590125    -3.722676      20.41
 C       2.624959     2.399626    -0.961417      69.19
 C       1.965958     3.716762    -0.487591      98.01
 H       2.358801     4.274880    -1.578030      20.71
 O       2.284000     4.277165     0.714061     282.91
 H       3.330398     4.199395     0.680308      25.89
 C       0.357541     3.659772    -0.503258      52.47
 H       0.170253     3.666137    -1.663177      17.20
 C      -0.225250     5.005691     0.217480      98.28
 O      -0.127701     6.183676    -0.634473     291.53
 H       0.115924     5.973928    -1.519405      31.52
 H       0.297663     5.054551     1.141247      23.79
 H      -1.296088     4.698912     0.420160      22.64
 C      -1.000564    -0.972653    -0.296074      39.84
 H      -0.157886    -1.763156    -0.003669      18.19
 C      -2.982714     0.250104    -0.678929      37.28
 H      -4.082467     0.102509    -0.773041      18.74
 C      -2.388712     1.599431    -0.306574     -11.37
 O      -2.886401     2.900501    -0.415828     204.95
 C      -4.042958     2.847519    -1.256271     103.39
 H      -4.880607     2.170904    -1.040563      25.48
 H      -4.389464     3.657124    -1.867311      25.29
 H      -3.905912     1.986363    -2.415072      21.94
 C      -0.945573     1.539445     0.107972      11.79
 O      -0.149271     2.635066     0.524351     144.27
 C      -0.381189     0.271530    -0.009511      27.48
 H       0.782320     0.085930     0.347792      16.71
 C      -2.342374    -1.024258    -0.751572      11.54
 C      -3.281545    -2.231066    -1.197192      77.62
 H      -4.110968    -1.980553    -1.889860      20.17
 O      -2.425424    -3.092613    -1.909475     295.06
 H      -2.975602    -3.818197    -1.980394      22.71
 C      -3.670095    -2.911999     0.138985      87.55
 H      -2.710169    -3.089445     0.841611      18.56
 O      -4.604038    -1.858050     0.882221     323.70
 H      -4.399215    -1.960684     1.906665      24.95
 C      -4.718387    -4.053810    -0.037803     112.68
 O      -4.308120    -5.046524    -1.073955     358.81
 H      -3.638876    -5.424494    -0.501809      31.65
 H      -5.568786    -3.453951    -0.389324      29.76
 H      -5.088785    -4.490475     0.704760      31.43
55
name = lig-etoh-frame_782
 C       2.529690     2.100803    -2.363128      49.94
 H       2.387550     2.819539    -3.103661      24.45
 C       3.021126     1.507548     0.081707      68.91
 H       3.340690     1.620276     1.135050      20.68
 C       3.323482     0.264871    -0.369410      10.90
 O       3.831152    -0.882592     0.534263     168.27
 C       4.373886    -0.487524     1.835222     111.97
 H       3.601792    -0.154938     2.714091      23.08
 H       5.209831     0.185884     1.659911      26.53
 H       4.721233    -1.449150     2.097260      25.15
 C       3.182005    -0.210737    -1.706528      22.13
 O       3.852696    -1.412739    -2.009106     139.38
 H       4.936461    -1.449294    -1.691048      23.57
 C       2.929268     0.752572    -2.749138      35.11
 H       2.969649     0.501203    -3.944969      19.05
 C       2.604762     2.361835    -0.938820      24.16
 C       2.080679     3.714690    -0.601442     107.46
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 H       2.341449     4.537146    -1.196937      23.34
 O       2.316550     4.304222     0.717672     304.82
 H       3.236333     4.497258     0.857273      30.53
 C       0.340337     3.680669    -0.440995      50.86
 H       0.194671     3.433884    -1.451870      20.01
 C      -0.206293     5.032203     0.172787      96.55
 O      -0.153980     6.164013    -0.658328     299.61
 H      -0.080154     5.888857    -1.663027      26.17
 H       0.437717     5.031860     1.155135      20.47
 H      -1.265588     4.911524     0.408557      22.72
 C      -1.021567    -1.053180    -0.205089      31.55
 H      -0.204976    -1.707572    -0.335479      18.99
 C      -2.945359     0.315565    -0.676537      46.23
 H      -4.014590     0.263258    -0.723432      20.16
 C      -2.367311     1.508970    -0.214500      -4.27
 O      -2.911625     2.906056    -0.428780     207.75
 C      -3.967963     2.814954    -1.306126     124.15
 H      -4.993857     2.422238    -0.915564      25.15
 H      -4.583683     3.827538    -1.608779      23.92
 H      -3.825242     2.239501    -2.011135      31.01
 C      -0.932854     1.570787     0.107491       9.92
 O      -0.155178     2.644884     0.505799     175.48
 C      -0.337987     0.234337     0.032468      13.88
 H       0.543736    -0.069005     0.347610      19.36
 C      -2.360761    -1.032129    -0.756147       4.28
 C      -3.255356    -2.232958    -1.156905      79.15
 H      -3.956013    -1.826310    -1.916860      19.61
 O      -2.418964    -3.047018    -1.922001     250.68
 H      -2.755888    -4.068970    -2.140728      18.29
 C      -3.678695    -2.926151     0.150611     103.40
 H      -2.911082    -3.180876     0.809886      22.29
 O      -4.602814    -1.848880     0.870077     332.62
 H      -4.430305    -1.897903     1.833282      28.45
 C      -4.735696    -4.049444    -0.071865      84.80
 O      -4.293593    -5.058777    -1.019317     261.93
 H      -3.351010    -5.472976    -0.675234      24.60
 H      -5.751812    -3.873263    -0.565878      24.44
 H      -5.136329    -4.696827     1.041435      24.05
55
name = lig-etoh-frame_783
 C       2.565989     2.086722    -2.311890      33.04
 H       2.215665     2.913479    -3.061153      19.81
 C       3.007333     1.575364     0.108741      58.32
 H       3.079352     1.754795     1.223762      16.45
 C       3.303918     0.279118    -0.471159       6.46
 O       3.852088    -0.843091     0.501339     168.80
 C       4.395982    -0.489455     1.830259     114.32
 H       3.818687    -0.248992     2.672899      26.33
 H       5.235156     0.270090     1.721216      26.48
 H       4.837757    -1.415969     2.430267      24.29
 C       3.238818    -0.228865    -1.798131      15.76
 O       3.881681    -1.449130    -2.022479     217.74
 H       4.680376    -1.515311    -1.647288      26.46
 C       2.930201     0.743970    -2.765423      54.23
 H       2.960245     0.397211    -3.701547      22.30
 C       2.566682     2.389458    -0.939874      47.50
 C       2.120691     3.755861    -0.639825      92.37
 H       2.270304     4.775862    -1.264543      21.67
 O       2.377951     4.318692     0.738992     264.33
 H       3.257242     4.743348     1.039542      31.02
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 C       0.355127     3.708483    -0.401525      44.01
 H      -0.193026     3.222763    -1.343787      17.68
 C      -0.193196     5.009133     0.134231     102.31
 O      -0.156580     6.168446    -0.701388     275.24
 H      -0.327609     5.844909    -1.656735      27.42
 H       0.384208     5.325944     0.956327      23.53
 H      -1.249049     4.936492     0.479367      23.00
 C      -1.042830    -1.072106    -0.166427      34.08
 H      -0.463038    -2.027392    -0.609621      17.61
 C      -2.934961     0.347205    -0.662467      51.97
 H      -4.027174     0.546112    -0.839526      20.28
 C      -2.286507     1.484520    -0.144036      -5.36
 O      -2.917175     2.866551    -0.417787     143.74
 C      -4.030314     2.837910    -1.328052      73.66
 H      -4.793484     2.536889    -0.597871      23.77
 H      -4.160163     3.917617    -1.389823      24.14
 H      -3.520005     2.083749    -2.432650      20.43
 C      -0.925746     1.518322     0.088862      11.59
 O      -0.152981     2.657295     0.488013     166.19
 C      -0.348035     0.188561     0.099167      14.16
 H       0.834007     0.076466     0.454664      15.39
 C      -2.357008    -0.979669    -0.718908       8.15
 C      -3.196889    -2.197227    -1.105323      73.23
 H      -4.093685    -1.730085    -1.604614      21.27
 O      -2.371559    -3.050442    -1.966771     271.09
 H      -2.724695    -3.977658    -2.062809      20.70
 C      -3.821229    -2.891406     0.175356      68.75
 H      -2.862449    -3.393455     0.809242      18.09
 O      -4.579060    -1.843767     0.807170     326.93
 H      -4.496234    -2.124229     1.907156      22.01
 C      -4.785615    -4.101279    -0.078032     105.63
 O      -4.245574    -5.095198    -0.970362     391.81
 H      -3.381176    -5.428503    -0.852759      31.34
 H      -5.723457    -3.909009    -0.575179      27.58
 H      -4.863147    -4.409093     0.818350      32.58
55
name = lig-etoh-frame_784
 C       2.600035     2.028382    -2.291211      49.00
 H       2.151460     2.751263    -2.880487      17.16
 C       2.997999     1.566955     0.085103      53.24
 H       2.838780     1.977835     1.058639      14.09
 C       3.318766     0.245507    -0.453619       5.87
 O       3.866644    -0.772806     0.460621     202.30
 C       4.456523    -0.504458     1.822798     102.53
 H       3.589476    -0.043112     2.559539      23.45
 H       5.160760     0.308396     1.808066      26.64
 H       4.944782    -1.331185     2.232003      26.72
 C       3.349084    -0.217373    -1.841282      12.27
 O       3.865012    -1.481637    -2.072879     140.54
 H       4.700903    -1.629382    -1.354251      19.78
 C       2.906047     0.759448    -2.753842      64.18
 H       2.933301     0.364739    -3.887830      23.06
 C       2.546322     2.477062    -0.946204      96.63
 C       2.078665     3.888082    -0.589259      83.65
 H       2.187647     4.477993    -1.544333      25.62
 O       2.441800     4.318156     0.768871     279.61
 H       3.391285     4.751734     0.872109      30.18
 C       0.360298     3.689526    -0.437570      65.08
 H      -0.281108     3.567048    -1.264756      19.53
 C      -0.205397     5.007038     0.121157      89.11
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 O      -0.154917     6.179159    -0.773732     246.77
 H      -0.413289     5.939229    -1.649959      31.98
 H       0.399231     5.543600     0.955002      23.51
 H      -1.208023     4.723493     0.543650      23.45
 C      -1.038990    -1.060811    -0.193590      58.06
 H      -0.830729    -2.083484    -0.423171      20.71
 C      -2.952870     0.359163    -0.630999      55.13
 H      -3.904288     0.610950    -1.054774      20.56
 C      -2.248128     1.542319    -0.142080      -3.47
 O      -2.872909     2.778546    -0.380098     185.96
 C      -4.060350     2.852091    -1.351717      99.93
 H      -4.860471     2.395611    -0.727131      24.26
 H      -3.771356     3.969526    -1.508233      22.75
 H      -3.918470     2.446634    -2.188568      30.10
 C      -0.866493     1.425309     0.092872      -0.39
 O      -0.142873     2.645828     0.505751     163.83
 C      -0.313478     0.119618     0.195127      52.54
 H       0.664764     0.341556     0.350727      19.11
 C      -2.356220    -0.889037    -0.642778      18.19
 C      -3.153523    -2.142777    -1.052059      68.83
 H      -4.139259    -1.830275    -1.440674      21.93
 O      -2.326275    -3.051023    -2.004758     261.45
 H      -2.873024    -3.844833    -1.928733      19.46
 C      -3.940100    -2.870859     0.173308      87.32
 H      -3.146071    -3.303122     0.700844      19.56
 O      -4.549770    -1.854129     0.777803     385.05
 H      -4.648474    -2.122584     1.643082      26.86
 C      -4.798708    -4.133428    -0.123397      54.22
 O      -4.216962    -5.142865    -0.957313     346.12
 H      -3.227356    -5.406542    -0.579243      22.76
 H      -5.787900    -3.714398    -0.493899      26.12
 H      -4.862778    -4.479547     1.158411      25.14
55
name = lig-etoh-frame_785
 C       2.597913     2.007181    -2.266731      58.78
 H       2.097047     2.678324    -3.084952      16.33
 C       2.970850     1.537438    -0.015801      43.75
 H       2.779119     1.991900     1.034813      14.01
 C       3.370582     0.216071    -0.359248      33.12
 O       3.892788    -0.709036     0.425362     233.71
 C       4.466055    -0.459588     1.802256      89.00
 H       3.572435    -0.127989     2.222874      25.67
 H       5.193428     0.431342     1.768808      24.95
 H       4.967049    -1.499563     1.968616      23.98
 C       3.464432    -0.177164    -1.809523      15.56
 O       3.859060    -1.496067    -2.129060     166.86
 H       4.321533    -1.848156    -1.249845      19.31
 C       2.897667     0.722124    -2.771599      62.94
 H       2.812890     0.653921    -3.830177      27.31
 C       2.571755     2.537054    -0.935727      82.63
 C       1.967137     3.957408    -0.520759      79.82
 H       2.167262     4.484300    -1.564516      24.30
 O       2.507820     4.325547     0.770614     321.67
 H       3.438108     4.504247     0.641444      33.74
 C       0.369003     3.700149    -0.468744      60.97
 H      -0.094776     3.807598    -1.556462      14.99
 C      -0.215356     5.048128     0.146023      94.30
 O      -0.160966     6.184993    -0.838004     219.93
 H      -0.414038     5.961713    -1.849871      27.64
 H       0.345661     5.340255     0.990321      25.46
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 H      -1.197545     4.687706     0.470106      23.04
 C      -1.032944    -1.023438    -0.224547      47.19
 H      -0.706115    -2.125633    -0.055369      19.72
 C      -2.962404     0.419497    -0.585870      42.41
 H      -3.871310     0.451935    -1.234776      19.84
 C      -2.247782     1.569260    -0.211767       9.74
 O      -2.815209     2.688728    -0.343207     159.95
 C      -4.040050     2.909209    -1.279561      87.13
 H      -5.098130     2.543986    -1.065888      23.56
 H      -4.088963     3.920301    -1.555240      25.44
 H      -4.225137     2.336892    -2.594851      21.45
 C      -0.815628     1.364758     0.124584      -2.15
 O      -0.118751     2.605379     0.531688     103.91
 C      -0.279024     0.065745     0.271996      49.97
 H       0.907771     0.205969     0.368192      16.89
 C      -2.376622    -0.829740    -0.562066      22.24
 C      -3.143113    -2.087060    -1.017347      66.73
 H      -3.984041    -1.816281    -1.747735      20.68
 O      -2.315340    -3.033363    -2.004907     179.71
 H      -3.066908    -3.843360    -1.865745      14.85
 C      -3.948168    -2.899875     0.107218      79.57
 H      -3.102276    -3.269899     0.966701      16.69
 O      -4.563088    -1.825411     0.751323     324.52
 H      -4.860402    -2.060618     1.820525      22.72
 C      -4.820139    -4.142432    -0.107309     104.17
 O      -4.179536    -5.186979    -0.947315     381.21
 H      -3.467929    -5.387214    -0.317392      30.18
 H      -5.800442    -3.806572    -0.452447      27.77
 H      -5.099783    -4.569470     0.726656      30.94
55
name = lig-etoh-frame_786
 C       2.544664     2.052184    -2.279878      65.25
 H       2.225407     2.553955    -3.152910      20.55
 C       2.935168     1.529061    -0.073549      58.22
 H       2.948401     1.664486     0.970006      17.37
 C       3.429472     0.246343    -0.347344      43.27
 O       3.948661    -0.693896     0.421557     252.08
 C       4.472377    -0.406379     1.721482     111.49
 H       3.509802    -0.278004     2.427860      24.31
 H       5.192386     0.369137     1.719744      27.32
 H       4.810911    -1.406926     1.931531      25.97
 C       3.540961    -0.142749    -1.755131      27.48
 O       3.841568    -1.487096    -2.168772     212.05
 H       4.037108    -1.967661    -1.414394      21.97
 C       2.912202     0.693469    -2.736854      64.18
 H       2.746238     0.671194    -3.863923      24.04
 C       2.606450     2.548582    -0.961814      29.66
 C       1.856334     3.910909    -0.484138      96.83
 H       2.131646     4.824341    -1.158598      19.88
 O       2.547511     4.346485     0.745019     274.39
 H       3.589744     4.213558     0.573142      27.12
 C       0.376276     3.773368    -0.483660      51.75
 H       0.271501     3.560867    -1.546044      17.46
 C      -0.237228     5.072686     0.136926      95.61
 O      -0.175048     6.187337    -0.879677     240.02
 H      -0.210240     5.794524    -1.779051      29.23
 H       0.362343     5.241495     1.104388      21.71
 H      -1.348637     4.912202     0.341848      21.61
 C      -1.014184    -1.013041    -0.211231      35.97
 H      -0.498407    -1.887780     0.230840      20.93
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 C      -2.981427     0.457378    -0.572059      52.12
 H      -3.886437     0.408249    -1.156005      19.87
 C      -2.191581     1.476606    -0.293508      10.69
 O      -2.820707     2.708909    -0.343561     185.83
 C      -4.039085     2.928722    -1.271762     110.91
 H      -5.053301     2.728354    -0.929197      26.01
 H      -4.311477     4.057202    -1.427968      24.51
 H      -3.977599     2.417533    -2.171523      27.69
 C      -0.802899     1.367711     0.169293      11.80
 O      -0.083113     2.555253     0.531740      57.13
 C      -0.208168     0.066531     0.312766      31.39
 H       0.808273    -0.299913     0.484231      19.58
 C      -2.385900    -0.841183    -0.495528      21.49
 C      -3.165472    -2.058267    -1.050490      74.84
 H      -3.724917    -1.655239    -1.879976      20.09
 O      -2.356441    -3.015692    -1.951230     271.64
 H      -2.801514    -3.809076    -2.018812      22.86
 C      -3.855842    -2.929691     0.104118      97.97
 H      -3.145349    -3.240851     0.797217      21.01
 O      -4.631476    -1.774308     0.740703     359.42
 H      -4.740820    -2.044736     1.648566      28.10
 C      -4.861185    -4.133530    -0.142605      84.38
 O      -4.173182    -5.200276    -0.931294     312.28
 H      -3.465892    -5.615145    -0.342763      26.73
 H      -5.807169    -3.937825    -0.724885      25.75
 H      -5.328029    -4.801712     0.879337      24.43
55
name = lig-etoh-frame_787
 C       2.500091     2.069279    -2.337459      81.90
 H       2.226043     2.757717    -3.193885      25.80
 C       2.930182     1.512254    -0.057240      92.21
 H       3.050394     1.555827     1.086511      20.47
 C       3.492662     0.311642    -0.453466      46.88
 O       4.011556    -0.711621     0.435529     251.77
 C       4.424084    -0.377689     1.668237     131.07
 H       3.851717    -0.295239     2.586464      26.82
 H       5.252643     0.421381     1.724371      26.65
 H       4.917674    -1.338234     2.103899      25.37
 C       3.554998    -0.140094    -1.741673       7.42
 O       3.817777    -1.433980    -2.209215     142.69
 H       3.887195    -2.220546    -1.395657      18.49
 C       2.936329     0.732009    -2.657683      73.40
 H       2.812552     0.303525    -3.725378      21.42
 C       2.592212     2.555484    -1.019741      38.50
 C       1.859907     3.837227    -0.442721     102.92
 H       1.951306     4.893075    -1.009204      15.12
 O       2.571300     4.358622     0.718298     313.71
 H       3.488009     4.053871     0.702737      28.07
 C       0.376419     3.827951    -0.459427      30.38
 H       0.200543     3.280914    -1.461024      17.67
 C      -0.287439     5.086139     0.092901     108.71
 O      -0.176953     6.183906    -0.884298     237.57
 H       0.008363     5.676479    -1.747703      25.80
 H       0.250769     5.347794     0.997632      23.50
 H      -1.313393     5.048773     0.278811      23.71
 C      -0.985700    -0.989320    -0.122397      52.14
 H      -0.545164    -1.956532     0.138019      21.25
 C      -2.997350     0.362576    -0.596443      36.93
 H      -4.047044     0.583553    -0.910268      17.44
 C      -2.114652     1.442505    -0.349792     -12.80
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 O      -2.846249     2.790926    -0.362508     151.96
 C      -4.055023     2.984566    -1.218910      81.16
 H      -4.866555     2.567654    -0.499693      22.81
 H      -4.037700     4.058552    -1.293019      23.97
 H      -3.471348     2.261667    -2.212030      19.16
 C      -0.773065     1.401393     0.209683      18.09
 O      -0.043236     2.516354     0.518530      68.65
 C      -0.184059     0.082092     0.303461      35.18
 H       0.746650    -0.351387     0.704239      19.41
 C      -2.371733    -0.906018    -0.461235      20.77
 C      -3.185640    -2.082561    -1.110874      70.55
 H      -3.895803    -1.458962    -1.793839      19.78
 O      -2.379413    -2.978976    -1.878955     259.64
 H      -2.741118    -3.932069    -2.032270      17.99
 C      -3.834310    -2.888949     0.100219      62.46
 H      -2.833356    -3.354575     0.750396      15.77
 O      -4.696280    -1.743630     0.706473     294.91
 H      -4.662038    -2.090829     1.737618      21.75
 C      -4.906199    -4.171010    -0.175183      86.19
 O      -4.192208    -5.200190    -0.918488     342.59
 H      -3.390621    -5.757575    -0.566513      26.16
 H      -5.617678    -3.894571    -0.980583      26.45
 H      -5.238523    -4.438494     0.723002      29.44
55
name = lig-etoh-frame_788
 C       2.477825     2.080265    -2.418181      54.89
 H       2.167221     2.874134    -3.109708      25.70
 C       2.961508     1.519575    -0.014957      83.34
 H       2.950595     1.774197     1.011742      22.66
 C       3.582370     0.337668    -0.510531      32.01
 O       4.037625    -0.725448     0.408950     230.82
 C       4.461253    -0.373116     1.715191     117.09
 H       3.713833    -0.053328     2.582687      24.22
 H       5.139494     0.461224     1.642337      27.14
 H       5.138059    -1.144847     2.074447      25.91
 C       3.512847    -0.152572    -1.785889      16.47
 O       3.796108    -1.382572    -2.233333     231.80
 H       3.840087    -2.043007    -1.531851      25.85
 C       2.956609     0.781963    -2.616996      51.90
 H       2.877530     0.179005    -3.491875      21.70
 C       2.535827     2.536278    -1.037803      48.38
 C       1.948353     3.805243    -0.428320      85.21
 H       1.828719     4.566113    -1.291545      17.24
 O       2.569051     4.356889     0.715722     316.89
 H       3.451770     4.002076     0.827844      27.28
 C       0.359597     3.788084    -0.410014      29.63
 H      -0.175672     3.382874    -1.313051      17.39
 C      -0.337000     5.108410     0.032531     103.10
 O      -0.165007     6.174375    -0.883272     232.08
 H       0.158212     5.851142    -1.836523      25.11
 H       0.164831     5.507508     0.957569      22.84
 H      -1.436401     4.854526     0.309738      22.00
 C      -0.985121    -0.996092    -0.005298      54.88
 H      -0.689485    -2.107861    -0.183131      18.96
 C      -2.963926     0.265565    -0.618997      32.03
 H      -4.012322     0.578368    -0.572378      17.90
 C      -2.104787     1.488964    -0.379576     -25.23
 O      -2.816153     2.860560    -0.366001     171.36
 C      -3.991519     2.979029    -1.143932     117.82
 H      -4.721863     2.444676    -0.572518      24.81
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 H      -3.939809     4.095546    -1.332969      23.93
 H      -3.820264     2.518488    -2.067044      26.77
 C      -0.745503     1.428981     0.210144       9.80
 O       0.004396     2.506623     0.526997      79.88
 C      -0.194125     0.103152     0.280556      35.03
 H       0.771733     0.099327     0.981776      15.45
 C      -2.353230    -0.985038    -0.483916      18.36
 C      -3.222843    -2.113938    -1.131734      86.20
 H      -4.089307    -1.656863    -1.566577      21.63
 O      -2.374472    -2.952960    -1.828722     248.76
 H      -2.910101    -3.888235    -1.794833      16.46
 C      -3.864300    -2.829778     0.080176      86.20
 H      -3.036270    -3.193291     0.600266      21.68
 O      -4.733638    -1.766873     0.691354     349.29
 H      -4.693705    -1.950819     1.734108      24.56
 C      -4.859959    -4.152000    -0.256629      64.31
 O      -4.225395    -5.221277    -0.933173     336.31
 H      -3.394428    -5.501434    -0.507476      28.76
 H      -5.574243    -3.731694    -0.973745      26.38
 H      -5.391067    -4.271613     0.926356      24.96
55
name = lig-etoh-frame_789
 C       2.473037     2.121406    -2.425898      53.02
 H       2.077991     2.767760    -3.204453      22.97
 C       3.014175     1.561082    -0.043080      87.77
 H       2.870065     1.971509     1.002330      16.62
 C       3.673126     0.324589    -0.447257      43.73
 O       4.046486    -0.730842     0.368148     237.62
 C       4.527534    -0.336926     1.795813      96.04
 H       3.569008    -0.007998     2.198297      23.12
 H       5.056901     0.654089     1.562884      26.04
 H       5.217995    -1.147493     2.089787      23.92
 C       3.447601    -0.120433    -1.802117      32.14
 O       3.782196    -1.341577    -2.272062     205.29
 H       3.910996    -1.885562    -1.482941      29.21
 C       2.954457     0.821070    -2.670088      70.80
 H       2.788117     0.326507    -3.768067      17.91
 C       2.483692     2.454748    -1.008778      33.91
 C       1.997565     3.788402    -0.490456      70.19
 H       2.120132     4.399693    -1.567622      18.91
 O       2.545443     4.351722     0.718166     284.91
 H       3.541084     4.036714     0.923338      26.21
 C       0.327623     3.691622    -0.331952      55.43
 H      -0.240384     3.612432    -1.302610      17.95
 C      -0.380029     5.105916     0.018813     107.16
 O      -0.142933     6.180638    -0.903407     264.67
 H       0.027141     5.969560    -1.795705      31.67
 H       0.004666     5.531524     0.969019      24.30
 H      -1.345563     4.687809     0.166132      23.90
 C      -1.024818    -1.083101     0.060146      41.37
 H      -0.543150    -1.977985    -0.203891      20.97
 C      -2.870986     0.281918    -0.603306      34.02
 H      -3.967792     0.291704    -0.481650      18.60
 C      -2.143801     1.546594    -0.377558      -4.06
 O      -2.712181     2.879842    -0.357743     207.82
 C      -3.901869     2.980943    -1.065296     122.11
 H      -4.919485     2.535500    -0.695584      24.21
 H      -4.275888     4.047810    -1.255695      24.84
 H      -4.334475     2.624697    -2.295197      22.25
 C      -0.776389     1.444685     0.144035      -2.27
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 O       0.059587     2.530256     0.564421     130.55
 C      -0.200588     0.157757     0.307922      27.34
 H       0.658209     0.329819     0.842495      16.60
 C      -2.335809    -1.017189    -0.543665      13.52
 C      -3.257688    -2.113948    -1.064751      78.39
 H      -4.209255    -1.838148    -1.710732      19.85
 O      -2.374723    -2.977325    -1.804125     288.00
 H      -2.852949    -3.732238    -1.716700      23.42
 C      -3.957725    -2.788745     0.042223      80.58
 H      -3.073878    -3.103318     0.911440      18.71
 O      -4.755131    -1.817854     0.685691     373.08
 H      -4.751792    -1.900140     1.611155      29.84
 C      -4.804468    -4.048986    -0.290932     104.10
 O      -4.259150    -5.248512    -0.953191     349.95
 H      -3.417168    -5.284562    -0.365537      28.64
 H      -5.681475    -3.638783    -0.870819      26.26
 H      -5.354884    -4.322295     0.512077      27.86
55
name = lig-etoh-frame_790
 C       2.480771     2.145882    -2.372400     101.50
 H       1.980696     2.638972    -3.265739      17.80
 C       3.089790     1.588085    -0.080634      73.18
 H       2.971289     1.938057     0.939422      11.17
 C       3.705457     0.312972    -0.383399      50.62
 O       4.080104    -0.739666     0.357940     267.33
 C       4.575754    -0.262848     1.789249      96.22
 H       3.554943    -0.192102     2.214681      22.69
 H       5.072185     0.693639     1.678032      26.89
 H       5.092430    -1.154930     2.274214      23.48
 C       3.392173    -0.038242    -1.776779      28.49
 O       3.767129    -1.319387    -2.310679     162.11
 H       4.212414    -1.801573    -1.372886      24.36
 C       2.912735     0.855122    -2.823401      34.60
 H       2.768359     0.707369    -3.816240      20.21
 C       2.451974     2.369456    -0.988987      46.94
 C       1.983769     3.777864    -0.599476      89.83
 H       2.484759     4.407776    -1.356658      24.29
 O       2.515938     4.335526     0.712342     312.33
 H       3.465431     4.267180     0.820686      33.06
 C       0.332062     3.634808    -0.279160      72.94
 H       0.006152     3.544155    -1.378634      17.35
 C      -0.388636     5.068323     0.046558      92.86
 O      -0.122882     6.198833    -0.907388     225.35
 H      -0.191054     5.777970    -1.925195      25.24
 H      -0.177227     5.459237     1.044722      24.69
 H      -1.518441     4.806677    -0.049176      22.05
 C      -1.040773    -1.145392     0.071241      21.53
 H      -0.209019    -1.983392     0.040030      17.77
 C      -2.796221     0.372468    -0.568189      53.65
 H      -3.875306     0.168920    -0.694257      18.32
 C      -2.169016     1.577830    -0.342700      23.06
 O      -2.600774     2.856780    -0.370446     205.29
 C      -3.952629     3.007772    -1.056480     121.42
 H      -4.763431     2.609199    -0.470132      26.35
 H      -4.285112     4.036485    -0.961535      26.10
 H      -4.020355     2.638649    -2.059349      26.69
 C      -0.825958     1.459515     0.056471       3.74
 O       0.091569     2.563210     0.597010     123.98
 C      -0.285846     0.195530     0.336480       2.70
 H       0.909955     0.195329     0.677906      12.92
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 C      -2.296404    -0.980079    -0.589351      16.24
 C      -3.276498    -2.089184    -1.017900      79.60
 H      -3.906324    -1.776227    -1.821182      21.12
 O      -2.376446    -3.017365    -1.787104     224.16
 H      -2.803693    -4.042453    -1.817711      15.67
 C      -4.002501    -2.804935     0.098813     106.85
 H      -3.341146    -3.073237     0.835810      22.89
 O      -4.803251    -1.853019     0.662423     321.62
 H      -4.750639    -2.025293     1.786734      22.92
 C      -4.807790    -3.929500    -0.360851      89.47
 O      -4.277530    -5.238892    -0.958725     288.43
 H      -3.429752    -5.509322    -0.440578      26.69
 H      -5.646283    -3.629215    -0.965109      25.28
 H      -5.384257    -4.495428     0.641063      23.96
55
name = lig-etoh-frame_791
 C       2.474597     2.108951    -2.358434      61.53
 H       1.943412     2.787177    -2.989254      16.81
 C       3.188805     1.566417    -0.061138      60.83
 H       3.204205     1.890335     0.977569      10.03
 C       3.654856     0.333346    -0.422658       6.97
 O       4.154443    -0.747233     0.397834     252.24
 C       4.565660    -0.224935     1.742906     115.52
 H       3.693001    -0.250370     2.490018      24.51
 H       5.188913     0.708312     1.830534      27.08
 H       5.043678    -1.016440     2.283451      25.53
 C       3.367237     0.021075    -1.808661      33.34
 O       3.763978    -1.291959    -2.293643     208.24
 H       4.427227    -1.653988    -1.795351      29.02
 C       2.869916     0.910483    -2.892257      64.53
 H       2.832429     0.794149    -4.120725      24.70
 C       2.432755     2.357152    -0.999412      77.50
 C       1.962550     3.763118    -0.619733     109.68
 H       2.415200     4.610131    -1.341230      25.77
 O       2.464824     4.307769     0.691958     241.70
 H       3.469912     4.503234     0.664171      33.19
 C       0.389265     3.670720    -0.314337      74.26
 H       0.111614     3.224015    -1.291579      18.25
 C      -0.413672     5.014767     0.063465     100.67
 O      -0.099287     6.186720    -0.913022     239.03
 H      -0.297191     5.713943    -1.714161      30.25
 H      -0.304467     5.364758     1.137426      25.11
 H      -1.437117     5.001159    -0.157113      24.27
 C      -0.981776    -1.126542     0.051337      33.49
 H      -0.382916    -1.936033     0.315342      20.38
 C      -2.792704     0.412619    -0.565250      63.03
 H      -3.802277     0.516846    -1.005445      19.97
 C      -2.152523     1.603354    -0.291487      20.22
 O      -2.545894     2.849003    -0.408120     186.16
 C      -4.025568     3.056699    -1.001836      83.31
 H      -4.556096     2.399454    -0.211571      23.61
 H      -4.002305     4.196275    -0.790418      23.19
 H      -3.479707     2.540807    -2.052301      19.83
 C      -0.801708     1.464466     0.029543       4.59
 O       0.081409     2.573959     0.604985     109.36
 C      -0.363333     0.171087     0.353913      36.79
 H       0.602258    -0.009286     0.423474      19.61
 C      -2.231700    -0.920505    -0.585533      16.32
 C      -3.221780    -2.078592    -1.016617      63.30
 H      -3.819379    -1.503584    -1.843514      20.68
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 O      -2.381094    -3.091628    -1.768688     269.45
 H      -2.740974    -3.991431    -1.869177      19.06
 C      -3.999346    -2.813958     0.135366      66.72
 H      -3.135809    -3.345045     0.947072      18.38
 O      -4.894686    -1.856879     0.696700     343.78
 H      -4.831095    -2.053745     1.586950      28.06
 C      -4.893159    -3.934264    -0.391426      88.80
 O      -4.279261    -5.199686    -0.970832     348.69
 H      -3.553889    -5.685808    -0.578370      29.89
 H      -5.597686    -3.602875    -1.219138      25.74
 H      -5.252673    -4.226141     0.525936      27.78
55
name = lig-etoh-frame_792
 C       2.417686     2.093508    -2.367736      36.22
 H       1.969445     3.053264    -2.794267      11.48
 C       3.249237     1.575667    -0.016624      65.07
 H       3.486906     1.915826     1.035935      11.00
 C       3.578629     0.316280    -0.519527      10.98
 O       4.237619    -0.711653     0.445598     201.73
 C       4.529948    -0.223254     1.722455     115.63
 H       3.770451    -0.015160     2.479669      26.76
 H       5.188726     0.689848     1.781068      27.56
 H       5.288031    -1.049144     2.083077      25.48
 C       3.377872     0.016312    -1.910604      17.65
 O       3.750498    -1.241527    -2.278978     136.75
 H       4.784686    -1.572382    -1.989188      19.23
 C       2.859209     0.923568    -2.920604      -1.31
 H       2.949880     0.654929    -3.862593      25.96
 C       2.472782     2.386704    -0.976967     120.56
 C       1.953892     3.783952    -0.559864     115.49
 H       1.858774     4.559128    -1.416174      24.86
 O       2.418414     4.267474     0.667093     244.09
 H       3.354498     4.708729     0.551335      30.79
 C       0.442383     3.725639    -0.407150      50.18
 H      -0.043315     3.129262    -1.257930      17.20
 C      -0.414717     4.981532     0.048800     100.79
 O      -0.067733     6.153127    -0.875988     225.85
 H      -0.235725     5.772987    -1.810245      27.12
 H      -0.261071     5.238004     1.073889      25.06
 H      -1.506079     4.781356    -0.158676      21.72
 C      -0.944003    -1.025686     0.018464      64.30
 H      -0.667413    -2.079099     0.409380      19.07
 C      -2.837037     0.413836    -0.613503      57.09
 H      -3.668066     0.775923    -1.224762      19.96
 C      -2.091027     1.614913    -0.240839      -1.83
 O      -2.534245     2.887490    -0.441191     175.77
 C      -3.981637     3.081738    -0.923405     121.21
 H      -4.551370     2.320799    -0.367564      25.41
 H      -4.019575     4.112870    -0.899442      26.42
 H      -3.854771     2.782217    -1.866483      28.21
 C      -0.714833     1.466876     0.084253      10.66
 O       0.046881     2.561948     0.600036      90.98
 C      -0.411081     0.117165     0.343576      50.91
 H       0.807285    -0.067333     0.484636      17.68
 C      -2.201056    -0.886284    -0.549072      16.97
 C      -3.119791    -2.065546    -1.045614      79.83
 H      -3.882844    -1.554917    -1.593387      22.60
 O      -2.374048    -3.146377    -1.749871     255.96
 H      -2.959752    -3.961481    -1.745687      17.16
 C      -3.948194    -2.818226     0.130990      85.70
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 H      -3.279530    -3.292263     0.747893      20.91
 O      -4.986322    -1.856605     0.734119     287.92
 H      -4.980769    -2.036483     1.796635      23.08
 C      -4.948898    -3.985534    -0.431954      67.45
 O      -4.297308    -5.143069    -1.012888     302.75
 H      -3.566758    -5.642170    -0.411842      25.93
 H      -5.541339    -3.605930    -1.241240      27.15
 H      -5.636750    -4.166141     0.647187      25.18
55
name = lig-etoh-frame_793
 C       2.327682     2.149842    -2.342609     103.57
 H       2.070289     2.986557    -2.972799      26.51
 C       3.266047     1.609874    -0.008390      60.05
 H       3.628060     1.941128     0.920910      19.50
 C       3.523923     0.289684    -0.573465      -8.58
 O       4.284453    -0.647039     0.426034     167.15
 C       4.559703    -0.231732     1.732437     113.01
 H       3.642969     0.109812     2.353459      24.86
 H       5.135565     0.723730     1.568328      26.10
 H       5.248387    -0.965282     1.973591      26.39
 C       3.401319    -0.005623    -1.991354      36.00
 O       3.765741    -1.232685    -2.284169     158.78
 H       4.787776    -1.305276    -2.118679      21.52
 C       2.872801     0.898707    -2.876416      25.89
 H       2.998157     0.449607    -4.007183      18.78
 C       2.569831     2.432652    -0.927539      49.65
 C       1.899209     3.793093    -0.504352      89.32
 H       1.752920     4.523797    -1.505806      18.70
 O       2.394560     4.251800     0.656419     278.20
 H       3.189411     4.694210     0.575324      30.39
 C       0.418907     3.718813    -0.488690      43.47
 H      -0.048157     3.479945    -1.417706      18.70
 C      -0.403099     4.950338    -0.026489     112.52
 O      -0.042463     6.101888    -0.815257     220.84
 H      -0.016877     5.978436    -1.866358      26.48
 H      -0.098075     5.208228     1.048258      22.63
 H      -1.382867     4.463589    -0.027165      21.18
 C      -0.986406    -1.004522    -0.023813      64.22
 H      -0.839706    -2.047553     0.250275      21.81
 C      -2.836007     0.446570    -0.676719      42.59
 H      -3.671126     0.614166    -1.389360      20.32
 C      -2.028017     1.593520    -0.221840      -5.53
 O      -2.546127     2.940393    -0.467423     179.61
 C      -3.870050     3.073780    -0.842124     114.31
 H      -4.744483     2.488887    -0.408203      24.69
 H      -4.326118     4.205200    -0.835769      23.19
 H      -4.483285     2.952219    -2.113592      22.03
 C      -0.661477     1.474903     0.183630      18.58
 O       0.016537     2.546718     0.598127      92.75
 C      -0.252187     0.134613     0.357661      58.81
 H       0.645868     0.098698     0.813549      23.12
 C      -2.264255    -0.862551    -0.544476      20.07
 C      -3.025470    -2.062848    -1.036323      84.49
 H      -3.989318    -1.726508    -1.601556      20.53
 O      -2.368667    -3.186974    -1.733250     212.40
 H      -3.215729    -3.853143    -1.563376      14.19
 C      -3.967260    -2.797510     0.078375      61.97
 H      -3.183975    -3.309850     0.986944      17.00
 O      -5.044668    -1.873613     0.773469     246.42
 H      -5.040854    -2.052349     1.831518      23.79
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 C      -4.982600    -4.018113    -0.413134      97.33
 O      -4.309529    -5.100088    -1.051999     339.27
 H      -3.731234    -5.324582    -0.334481      31.96
 H      -5.616193    -3.547910    -1.225409      26.50
 H      -5.836441    -4.207313     0.155832      27.71
55
name = lig-etoh-frame_794
 C       2.293757     2.169542    -2.302535     107.71
 H       2.034655     2.828940    -3.177741      29.28
 C       3.263818     1.605029    -0.071855      59.45
 H       3.666530     2.004838     0.925191      21.00
 C       3.517644     0.305243    -0.534867       9.24
 O       4.282839    -0.589390     0.315057     195.11
 C       4.594879    -0.175326     1.719174      97.01
 H       3.674238    -0.064722     2.240301      26.54
 H       5.159943     0.789679     1.592531      24.57
 H       5.200393    -1.057688     2.263917      24.50
 C       3.407432    -0.008840    -1.958757      32.28
 O       3.812054    -1.279184    -2.331089     205.48
 H       4.700393    -1.328538    -2.104880      26.26
 C       2.866260     0.898707    -2.851411      34.61
 H       2.809439     0.633176    -3.856169      19.80
 C       2.635807     2.517428    -0.928657      59.60
 C       1.840725     3.774412    -0.528410     113.29
 H       2.209426     4.470011    -1.312783      21.41
 O       2.371355     4.266789     0.694175     276.11
 H       3.304131     4.678672     0.608826      28.22
 C       0.344545     3.672350    -0.529651      47.60
 H       0.071511     3.635098    -1.675861      19.23
 C      -0.352166     4.897718    -0.075515     117.98
 O      -0.022797     6.073370    -0.763353     265.25
 H       0.079264     5.926075    -1.671855      33.47
 H      -0.004926     5.183837     0.883545      24.49
 H      -1.403540     4.563263     0.021914      23.11
 C      -1.041505    -0.992921    -0.046940      -3.51
 H      -0.646478    -2.032537     0.110531      20.14
 C      -2.787385     0.500341    -0.745595      56.82
 H      -3.697130     0.449267    -1.331577      22.03
 C      -2.018214     1.560453    -0.260110       4.12
 O      -2.551963     2.966142    -0.492766     180.28
 C      -3.888099     3.106425    -0.843209     136.76
 H      -4.635433     2.585317    -0.169233      26.44
 H      -4.187973     4.044055    -0.535861      27.77
 H      -4.301695     2.981815    -1.831211      27.47
 C      -0.685571     1.455021     0.274819      11.02
 O       0.011428     2.569149     0.592840      88.47
 C      -0.065614     0.165018     0.381014      -8.26
 H       0.826059     0.081899     1.196634      17.32
 C      -2.349559    -0.824362    -0.570585      30.79
 C      -3.040071    -2.080067    -1.014846      90.44
 H      -3.721821    -1.789502    -1.793816      21.97
 O      -2.382922    -3.211937    -1.701720     264.29
 H      -2.969560    -3.921233    -1.680083      21.31
 C      -4.024148    -2.800444     0.115981      93.50
 H      -3.406173    -3.113927     0.863953      22.59
 O      -5.067569    -1.903724     0.790755     308.28
 H      -4.933410    -2.177388     1.691446      26.77
 C      -5.016780    -3.960663    -0.458331      82.07
 O      -4.319542    -5.062697    -1.078700     310.95
 H      -3.645337    -5.341480    -0.384311      28.62
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 H      -5.545075    -3.434216    -1.243843      26.10
 H      -5.965989    -4.429760     0.227301      24.63
55
name = lig-etoh-frame_795
 C       2.339185     2.131902    -2.287313      58.89
 H       1.820705     2.747529    -3.059694      25.98
 C       3.261075     1.616561    -0.132140      77.65
 H       3.490039     1.957969     0.826867      22.03
 C       3.564650     0.335051    -0.476438      39.66
 O       4.272252    -0.546896     0.191309     203.94
 C       4.633154    -0.129630     1.672634     113.24
 H       3.614843    -0.142302     2.241461      25.33
 H       5.204361     0.784639     1.821743      28.07
 H       5.027180    -0.896536     2.235132      28.09
 C       3.402094    -0.027351    -1.864714      43.24
 O       3.853893    -1.329821    -2.401299      85.21
 H       4.859520    -1.629314    -1.871595      20.81
 C       2.823404     0.946492    -2.782863      36.19
 H       2.604258     0.791686    -3.928253      19.04
 C       2.625563     2.593194    -1.001662      44.17
 C       1.878259     3.763114    -0.552978     121.89
 H       2.396329     4.590562    -1.289572      17.41
 O       2.343944     4.302795     0.768086     248.01
 H       3.350351     4.488789     0.606488      27.73
 C       0.287711     3.607719    -0.576686      63.62
 H       0.078925     3.265966    -1.550167      21.79
 C      -0.320105     4.850727    -0.058873      97.68
 O      -0.001007     6.077760    -0.727021     240.54
 H       0.106654     5.766836    -1.757580      26.17
 H       0.077034     5.021177     1.002410      22.42
 H      -1.431943     4.935316    -0.051578      22.90
 C      -1.024212    -0.948177    -0.022801      -0.64
 H      -0.433785    -1.919911    -0.093931      19.70
 C      -2.752338     0.522824    -0.821551      60.10
 H      -3.809456     0.668145    -1.187762      22.11
 C      -2.044826     1.582105    -0.335294       2.71
 O      -2.515539     2.941710    -0.509208     154.91
 C      -3.967487     3.148520    -0.782475      83.80
 H      -4.414528     2.417979    -0.037001      23.70
 H      -3.962881     4.266510    -0.382219      22.38
 H      -3.945438     2.829454    -2.095480      20.37
 C      -0.722117     1.405328     0.334352      -4.48
 O       0.016535     2.628345     0.568654      69.77
 C       0.019373     0.159396     0.409919       1.56
 H       0.839614    -0.114309     1.052262      17.50
 C      -2.338414    -0.815423    -0.582465      22.00
 C      -3.165051    -2.126491    -1.010360      64.93
 H      -3.621099    -1.668558    -1.981764      19.65
 O      -2.356676    -3.210599    -1.661344     216.75
 H      -2.847766    -4.159884    -1.780291      16.08
 C      -4.148632    -2.788984     0.143802      63.80
 H      -3.283418    -3.179347     1.051753      17.48
 O      -5.064441    -1.935126     0.776384     275.61
 H      -4.845800    -2.278795     1.834976      19.97
 C      -5.062320    -3.878151    -0.504691      86.87
 O      -4.319892    -5.030583    -1.100780     303.52
 H      -3.533459    -5.536494    -0.628522      25.44
 H      -5.559919    -3.348048    -1.334961      25.57
 H      -5.528668    -4.357858     0.311709      26.38
55
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name = lig-etoh-frame_796
 C       2.383404     2.130625    -2.302157       8.03
 H       1.661655     2.746331    -2.828166      21.98
 C       3.234292     1.699111    -0.174674      84.87
 H       3.310767     1.972883     0.927474      18.36
 C       3.614606     0.377700    -0.514823      51.71
 O       4.311462    -0.535071     0.157725     217.39
 C       4.603374    -0.107175     1.602141     107.04
 H       3.681160     0.053657     2.078061      28.05
 H       5.212186     0.854864     1.823946      27.76
 H       5.176839    -1.065040     2.006082      25.10
 C       3.390298    -0.065523    -1.825732      33.24
 O       3.920083    -1.352432    -2.437840     215.79
 H       4.439122    -1.788356    -1.844112      30.71
 C       2.792715     0.923194    -2.713831      77.56
 H       2.534003     0.754191    -3.781343      24.34
 C       2.603353     2.583100    -1.057726      46.14
 C       1.966691     3.821962    -0.559516     106.74
 H       2.010230     4.693198    -1.267439      20.87
 O       2.317090     4.326475     0.829956     279.31
 H       3.241470     4.317017     0.778198      33.06
 C       0.290246     3.524903    -0.587154      49.21
 H      -0.126786     2.818517    -1.436790      18.44
 C      -0.325735     4.862743     0.003535      92.16
 O       0.045747     6.090488    -0.732505     250.51
 H       0.073250     5.845536    -1.683250      28.49
 H       0.044468     4.762655     1.005497      24.66
 H      -1.392861     4.922527    -0.060963      23.99
 C      -0.928777    -0.897839     0.005574      49.88
 H      -0.500997    -1.851093    -0.179719      21.76
 C      -2.775890     0.506942    -0.889610      45.88
 H      -3.754182     0.875635    -1.099681      22.50
 C      -2.039603     1.644401    -0.398474      -7.52
 O      -2.454005     2.889648    -0.511730     159.04
 C      -3.974681     3.176789    -0.730602     104.17
 H      -4.464226     2.303261    -0.190538      24.10
 H      -4.043800     4.237076    -0.662649      25.15
 H      -4.041899     2.953829    -1.788313      25.34
 C      -0.719547     1.394087     0.346622      -4.36
 O       0.010196     2.671462     0.539803     115.41
 C      -0.073024     0.131918     0.406885      35.44
 H       0.959524    -0.190985     0.816712      16.77
 C      -2.256151    -0.845936    -0.583845      -3.57
 C      -3.303117    -2.150264    -1.037217      60.10
 H      -3.841679    -1.682350    -1.823282      21.69
 O      -2.307508    -3.202004    -1.613201     213.48
 H      -2.893958    -4.026812    -1.666911      17.73
 C      -4.208798    -2.788947     0.143076     103.24
 H      -3.515556    -3.260418     0.748848      22.63
 O      -5.055410    -1.958004     0.802056     379.78
 H      -5.041687    -1.984117     1.707449      30.59
 C      -5.027592    -3.822631    -0.532938      82.07
 O      -4.317184    -5.009730    -1.155274     326.22
 H      -3.624896    -5.427342    -0.677623      30.25
 H      -5.762621    -3.457587    -1.305764      24.92
 H      -5.573573    -4.216747     0.455448      24.93
55
name = lig-etoh-frame_797
 C       2.389708     2.177335    -2.350753      23.40
 H       1.580501     2.760944    -2.916533      19.74
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 C       3.221304     1.771269    -0.157134      65.34
 H       3.175025     2.029492     0.884800      16.91
 C       3.656296     0.436911    -0.613695      10.62
 O       4.384537    -0.524360     0.200857     225.59
 C       4.591837    -0.123121     1.521190     119.36
 H       3.594984     0.172555     2.048345      24.72
 H       5.184704     0.767506     1.493994      28.07
 H       5.174354    -0.960062     1.758563      25.60
 C       3.383447    -0.110898    -1.874962      14.20
 O       3.947610    -1.319777    -2.457112     192.83
 H       4.268825    -1.933424    -1.616915      23.45
 C       2.779258     0.809810    -2.676948      85.66
 H       2.582200     0.461666    -3.708033      25.67
 C       2.605910     2.570440    -1.032414      77.67
 C       1.985664     3.903780    -0.549103      81.80
 H       1.837147     4.803455    -1.300384      20.95
 O       2.280341     4.329258     0.851713     255.50
 H       3.322118     4.234210     1.108759      28.79
 C       0.320456     3.452909    -0.558819      66.42
 H      -0.141848     2.968480    -1.376358      20.93
 C      -0.344336     4.881456     0.008648      79.83
 O       0.105153     6.106524    -0.722737     213.65
 H       0.041065     5.918070    -1.710359      27.52
 H       0.038042     4.842247     1.065981      23.64
 H      -1.455833     4.666116     0.053022      22.54
 C      -0.875415    -0.919748    -0.015924      51.00
 H      -0.491657    -2.019140    -0.081764      19.80
 C      -2.768387     0.481701    -0.899792      30.49
 H      -3.828710     0.703449    -1.259771      21.38
 C      -1.981176     1.612059    -0.427939       1.51
 O      -2.422958     2.883814    -0.510701     160.31
 C      -3.904018     3.155072    -0.690144      98.47
 H      -4.679427     2.539922    -0.185019      25.07
 H      -4.251254     4.263168    -0.639900      23.87
 H      -4.443914     3.026411    -1.939390      22.17
 C      -0.712311     1.461692     0.294480       8.10
 O      -0.006489     2.655534     0.552251     176.91
 C      -0.208811     0.133651     0.416086      63.14
 H       0.942795     0.062074     0.403734      18.92
 C      -2.210308    -0.849038    -0.606706     -11.36
 C      -3.336408    -2.125759    -1.035433      54.40
 H      -4.186750    -1.780548    -1.760734      19.99
 O      -2.290306    -3.167914    -1.551440     193.90
 H      -2.907349    -3.922510    -1.602520      18.29
 C      -4.197703    -2.777388     0.072100      71.81
 H      -3.423484    -3.591776     0.748952      17.53
 O      -5.080220    -1.932330     0.819070     322.62
 H      -5.037637    -1.834479     1.855375      25.22
 C      -5.026542    -3.857343    -0.529420     108.73
 O      -4.332750    -4.969549    -1.227002     286.01
 H      -3.658585    -5.291132    -0.481403      27.15
 H      -5.841839    -3.602425    -1.175239      26.15
 H      -5.781570    -4.120189     0.238017      26.56
55
name = lig-etoh-frame_798
 C       2.380750     2.174221    -2.413784      55.01
 H       1.807735     2.677944    -3.147765      21.00
 C       3.249674     1.744638    -0.112501      56.88
 H       3.231953     2.074561     0.935347      17.84
 C       3.719091     0.470833    -0.656765      -8.75
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 O       4.422740    -0.495628     0.194722     230.55
 C       4.585454    -0.116063     1.458933     107.85
 H       3.722763     0.036601     2.079910      26.15
 H       5.290337     0.812528     1.310599      24.29
 H       5.197193    -0.953336     2.033711      24.31
 C       3.412626    -0.148448    -1.927329      20.26
 O       3.953959    -1.267928    -2.439440     207.54
 H       4.129070    -1.893704    -1.576097      22.96
 C       2.723571     0.742996    -2.718767      61.33
 H       2.601763     0.157958    -3.743967      23.76
 C       2.594411     2.641330    -1.025648      68.74
 C       1.945655     3.937532    -0.518662      85.76
 H       2.025017     4.828559    -1.279344      21.08
 O       2.253955     4.320614     0.845331     312.20
 H       3.157612     4.258661     1.227621      29.78
 C       0.371854     3.498484    -0.478556      57.34
 H       0.007381     3.288519    -1.581765      20.07
 C      -0.352487     4.874466    -0.018822      94.17
 O       0.151560     6.106450    -0.696488     170.65
 H      -0.039223     5.966349    -1.739381      25.87
 H       0.029477     5.193711     0.965734      24.00
 H      -1.400568     4.649256     0.065715      23.98
 C      -0.923761    -1.058896    -0.091447      15.66
 H      -0.415861    -1.938892     0.128612      22.07
 C      -2.722004     0.443087    -0.864741      59.78
 H      -3.631794     0.370410    -1.414680      21.61
 C      -1.934404     1.524882    -0.436105      19.26
 O      -2.457739     2.921809    -0.520118     172.58
 C      -3.858818     3.132406    -0.715811     116.57
 H      -4.651517     2.714755     0.019459      25.02
 H      -4.084819     4.186608    -0.380190      25.26
 H      -4.346418     2.975198    -1.815992      24.29
 C      -0.740511     1.525468     0.192599      15.93
 O      -0.020045     2.588441     0.603479     169.58
 C      -0.266741     0.220725     0.414630      23.42
 H       0.801089     0.271794     0.344967      21.90
 C      -2.242067    -0.831145    -0.655655      13.51
 C      -3.268470    -2.058514    -1.014279      80.97
 H      -4.035216    -1.900357    -1.759231      21.72
 O      -2.316217    -3.105716    -1.485533     213.24
 H      -2.853541    -4.042230    -1.679524      15.28
 C      -4.130795    -2.809504     0.048884      89.51
 H      -3.487670    -3.352072     0.705257      22.47
 O      -5.116996    -1.884408     0.826091     320.71
 H      -4.676912    -2.017704     1.802138      23.86
 C      -5.103707    -3.926460    -0.551226      84.61
 O      -4.342531    -4.919875    -1.265124     298.97
 H      -3.762632    -5.318163    -0.546008      28.90
 H      -5.791354    -3.470209    -1.350920      25.08
 H      -5.807212    -4.358434     0.275968      26.07
55
name = lig-etoh-frame_799
 C       2.387552     2.101811    -2.436618      66.44
 H       2.086072     2.716419    -3.391923      22.10
 C       3.273834     1.691928    -0.118365      79.14
 H       3.483430     1.981204     0.951906      22.15
 C       3.788144     0.467816    -0.635997      14.02
 O       4.422446    -0.482463     0.109598     245.51
 C       4.663700    -0.086176     1.478660     117.75
 H       3.686597     0.036160     2.095054      24.74
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 H       5.217122     0.802669     1.582767      28.60
 H       5.107474    -0.766798     2.166204      27.08
 C       3.444781    -0.087795    -1.928612      24.18
 O       3.948222    -1.246904    -2.399449     248.45
 H       4.212137    -1.770699    -1.738962      29.72
 C       2.657193     0.720302    -2.814054      46.20
 H       2.471290     0.323563    -3.759102      24.89
 C       2.596526     2.689180    -1.066039      74.10
 C       1.901455     3.909401    -0.466628     102.28
 H       2.171311     4.792993    -1.210751      19.08
 O       2.214543     4.314327     0.838146     312.05
 H       3.172789     4.299010     1.021459      29.38
 C       0.417458     3.663485    -0.398694      61.88
 H       0.245836     3.456360    -1.438895      22.12
 C      -0.320943     4.886661    -0.026836     109.91
 O       0.168232     6.089615    -0.698975     218.46
 H       0.005479     6.055671    -1.602305      31.02
 H      -0.046089     5.251317     0.966560      24.60
 H      -1.437202     4.837474    -0.111097      24.64
 C      -0.991203    -1.103204    -0.141113       8.66
 H      -0.407816    -2.008987     0.258632      22.00
 C      -2.667268     0.401997    -0.830571      74.41
 H      -3.553222     0.426363    -1.523567      23.57
 C      -2.002489     1.537601    -0.470644      19.40
 O      -2.502891     2.928793    -0.537950     167.42
 C      -3.845627     3.135535    -0.697831     110.28
 H      -4.327007     2.488332     0.015319      25.98
 H      -3.790264     4.205589    -0.412728      24.51
 H      -4.142647     2.842607    -1.908517      23.01
 C      -0.759208     1.505364     0.103523      23.06
 O      -0.012753     2.535119     0.641797      81.24
 C      -0.302756     0.246327     0.354034       5.58
 H       0.882001     0.266204     0.682234      21.53
 C      -2.278365    -0.899355    -0.684918      35.14
 C      -3.159630    -2.018834    -0.992254      92.65
 H      -3.758764    -1.708487    -1.945649      21.58
 O      -2.341414    -3.057708    -1.438425     283.69
 H      -2.783684    -3.814921    -1.642071      23.22
 C      -4.130900    -2.819587     0.046277      59.40
 H      -3.307439    -3.116279     0.994687      18.97
 O      -5.103782    -1.861347     0.830982     340.75
 H      -4.697827    -2.081892     1.599226      28.17
 C      -5.193500    -3.953543    -0.588622      85.82
 O      -4.347522    -4.891884    -1.292757     312.19
 H      -3.801128    -5.458204    -0.764559      29.47
 H      -5.659173    -3.366132    -1.322177      27.23
 H      -5.608504    -4.572399     0.255294      25.29
55
name = lig-etoh-frame_800
 C       2.394963     2.048218    -2.447148      78.54
 H       2.253615     2.730004    -3.213826      25.90
 C       3.283835     1.679644    -0.181253      93.56
 H       3.633984     1.901492     0.785506      23.87
 C       3.813628     0.468927    -0.628252      25.10
 O       4.446983    -0.488678     0.058709     202.63
 C       4.713990    -0.049679     1.544311      91.40
 H       3.688563     0.133239     1.854288      25.02
 H       5.222549     0.980646     1.804338      25.29
 H       5.247491    -0.937613     2.040644      26.04
 C       3.445418     0.035583    -1.930388      24.53
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 O       3.926828    -1.239857    -2.375906     137.29
 H       4.606080    -1.806617    -1.629372      19.69
 C       2.642546     0.733622    -2.850939      50.14
 H       2.325323     0.549645    -4.011911      22.32
 C       2.632568     2.615552    -1.107629      44.14
 C       1.887123     3.871036    -0.428099     109.46
 H       2.140415     4.740790    -1.164701      18.87
 O       2.205821     4.305995     0.861557     263.25
 H       3.257180     4.424381     0.741207      26.33
 C       0.442606     3.804933    -0.344390      48.18
 H       0.146362     3.348807    -1.354664      22.02
 C      -0.311075     4.970749     0.005211     117.91
 O       0.184032     6.086208    -0.704723     225.79
 H       0.054532     6.031955    -1.761928      23.76
 H      -0.243657     5.042209     1.143759      24.01
 H      -1.351439     4.915878    -0.333223      24.13
 C      -1.000215    -1.042966    -0.121465      64.19
 H      -0.697341    -2.037614     0.147607      24.94
 C      -2.689330     0.389605    -0.854500      58.80
 H      -3.558708     0.702633    -1.423254      26.83
 C      -2.109329     1.641582    -0.511354       4.78
 O      -2.486273     2.883828    -0.562127     182.76
 C      -3.843167     3.135432    -0.677478     103.78
 H      -4.294961     2.244783    -0.081711      23.35
 H      -3.952860     4.314482    -0.628594      23.20
 H      -4.176015     2.867875    -1.942485      22.66
 C      -0.750394     1.458204     0.047334     -24.78
 O       0.009197     2.522927     0.643302      50.89
 C      -0.288176     0.151178     0.267834      56.26
 H       0.519270     0.077032     0.925700      25.43
 C      -2.249905    -0.986607    -0.651147      24.90
 C      -3.136718    -2.029754    -1.021579      98.51
 H      -3.573243    -1.486006    -1.865926      21.33
 O      -2.302322    -3.032665    -1.415800     249.78
 H      -3.014156    -3.829170    -1.603454      14.76
 C      -4.166817    -2.768780     0.098055      77.74
 H      -3.453969    -3.107362     0.789599      22.27
 O      -5.063683    -1.857137     0.794908     286.94
 H      -4.913769    -2.063367     1.931585      23.14
 C      -5.162865    -3.956406    -0.583623      83.32
 O      -4.354456    -4.882393    -1.356190     258.63
 H      -3.802101    -5.607869    -0.809993      25.05
 H      -5.892977    -3.349559    -1.264747      25.19
 H      -5.717025    -4.476567     0.197880      27.56
55
name = lig-etoh-frame_801
 C       2.398721     2.062252    -2.418364      77.78
 H       2.081671     2.909977    -3.148880      23.13
 C       3.303058     1.697110    -0.259151      52.78
 H       3.607001     2.101509     0.776487      21.40
 C       3.787366     0.480844    -0.674889      22.47
 O       4.516957    -0.489953     0.075875     180.85
 C       4.747890    -0.022359     1.594090     105.31
 H       3.683711     0.086059     1.870966      25.90
 H       5.290285     0.864419     1.683060      28.29
 H       5.262500    -0.974061     1.767641      26.47
 C       3.450685     0.072271    -1.967582      25.15
 O       3.908841    -1.246787    -2.330815     169.04
 H       4.736570    -1.367627    -1.858621      27.25
 C       2.670072     0.779012    -2.881379      58.07
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 H       2.587976     0.555423    -3.843220      27.89
 C       2.658866     2.482221    -1.113735      46.18
 C       1.914054     3.834087    -0.434131      99.30
 H       2.043360     4.743325    -1.212179      19.96
 O       2.268284     4.294409     0.897548     276.92
 H       3.159993     4.604688     0.867253      30.16
 C       0.420676     3.794509    -0.362850      45.85
 H      -0.116815     3.339819    -1.216256      21.30
 C      -0.354180     5.082504     0.060492     118.25
 O       0.214432     6.129788    -0.722206     257.12
 H       0.141141     5.810964    -1.678654      27.13
 H      -0.442995     5.107870     1.121828      25.73
 H      -1.347505     4.820466    -0.342824      23.87
 C      -0.982537    -0.998681    -0.068358      70.83
 H      -0.750109    -2.070035     0.097318      24.39
 C      -2.763660     0.427813    -0.903757      42.95
 H      -3.783076     0.611053    -1.328195      25.17
 C      -2.088854     1.630361    -0.513780      10.77
 O      -2.460435     2.886773    -0.595197     215.80
 C      -3.876606     3.116866    -0.711777     132.68
 H      -4.539146     2.496247    -0.147067      27.92
 H      -4.270048     4.102012    -0.584119      27.51
 H      -4.276234     2.993819    -1.752765      26.85
 C      -0.744045     1.427896     0.011163     -34.50
 O       0.028356     2.527637     0.619329      41.29
 C      -0.264657     0.055239     0.182619      42.28
 H       0.374618    -0.159421     1.197402      22.26
 C      -2.229926    -0.927240    -0.592063      13.56
 C      -3.185628    -2.044834    -1.047214      81.25
 H      -3.806879    -1.564559    -1.869180      21.94
 O      -2.250782    -3.088113    -1.433335     230.97
 H      -2.927467    -3.823607    -1.563146      18.75
 C      -4.239709    -2.690109     0.120313      66.21
 H      -3.393566    -3.470802     0.732272      19.77
 O      -5.015942    -1.856273     0.790753     338.62
 H      -5.223250    -2.015051     1.659076      30.06
 C      -5.085251    -3.906440    -0.558267     102.98
 O      -4.358969    -4.891115    -1.433750     277.03
 H      -3.923681    -5.468616    -0.797655      29.40
 H      -5.934318    -3.591092    -1.128122      27.30
 H      -5.867984    -4.333632     0.221156      27.21
55
name = lig-etoh-frame_802
 C       2.373397     2.147926    -2.422977      60.78
 H       1.774359     2.826745    -2.981078      21.54
 C       3.378779     1.705499    -0.245413      53.01
 H       3.437197     2.232121     0.653268      20.05
 C       3.770340     0.454144    -0.713985       5.04
 O       4.588045    -0.448210     0.113979     182.86
 C       4.753369    -0.041943     1.559649     102.56
 H       3.793307    -0.015449     2.200744      26.30
 H       5.481580     0.860986     1.543611      25.67
 H       5.283694    -0.936032     1.907836      26.96
 C       3.464329     0.011750    -2.021245      26.25
 O       3.883464    -1.231316    -2.297866     176.39
 H       4.835820    -1.189798    -1.951676      25.40
 C       2.741955     0.851850    -2.877419      63.40
 H       2.804475     0.370393    -3.999832      25.17
 C       2.609119     2.443447    -1.104673      61.53
 C       1.963275     3.803992    -0.475558      92.33
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 H       2.076374     4.662165    -1.233152      22.98
 O       2.347923     4.270870     0.924788     249.75
 H       3.218243     4.739559     1.042985      29.44
 C       0.349407     3.692954    -0.369539      45.62
 H      -0.157238     3.487317    -1.334671      21.14
 C      -0.410147     5.136185     0.080904      93.35
 O       0.242482     6.189702    -0.728887     229.05
 H       0.234385     5.825487    -1.633357      28.94
 H      -0.454188     5.511598     1.186769      23.61
 H      -1.451268     4.864808    -0.223780      23.46
 C      -1.015644    -1.074453    -0.041719      15.07
 H      -0.531648    -2.070713     0.206993      22.21
 C      -2.843363     0.469777    -0.934159      60.34
 H      -3.889094     0.325299    -1.202727      23.30
 C      -1.987641     1.517806    -0.506400       7.69
 O      -2.477180     2.947602    -0.629670     131.70
 C      -3.938037     3.099943    -0.754009      90.08
 H      -4.688546     2.561942    -0.028605      24.23
 H      -4.298059     4.176968    -0.300099      23.51
 H      -4.376172     2.923534    -2.052469      22.30
 C      -0.712393     1.402617     0.004206       9.76
 O       0.031397     2.524786     0.574467      96.81
 C      -0.182191     0.080723     0.193552       9.61
 H       0.488429    -0.070477     0.917343      24.37
 C      -2.318660    -0.777978    -0.591282       5.51
 C      -3.231001    -2.041162    -1.032653      71.86
 H      -3.981217    -1.927357    -1.856825      22.18
 O      -2.221733    -3.158877    -1.467013     207.13
 H      -2.692966    -4.006633    -1.627630      21.10
 C      -4.223808    -2.729403     0.084643      88.76
 H      -3.582262    -3.327254     0.714768      23.37
 O      -5.000927    -1.804342     0.774375     308.40
 H      -5.316938    -2.196144     1.702682      26.32
 C      -5.055759    -3.841801    -0.533106     100.67
 O      -4.373593    -4.888276    -1.477395     277.37
 H      -3.889231    -5.437908    -0.825698      29.55
 H      -5.849817    -3.546221    -1.294866      26.22
 H      -5.527299    -4.357708     0.291368      29.31
55
name = lig-etoh-frame_803
 C       2.325662     2.210220    -2.456008      53.87
 H       1.496430     2.763812    -2.998361      20.32
 C       3.448996     1.703659    -0.223509      61.91
 H       3.497475     2.159025     0.832372      16.01
 C       3.790566     0.415602    -0.685009       6.15
 O       4.628913    -0.385888     0.145958     224.04
 C       4.782540    -0.083754     1.500069     126.94
 H       4.007699     0.067142     2.251232      28.19
 H       5.392473     0.793879     1.580123      28.41
 H       5.361666    -0.837896     2.137403      26.72
 C       3.459526    -0.016122    -2.029185      16.98
 O       3.872048    -1.244104    -2.294171     139.96
 H       4.948343    -1.422581    -2.004747      22.06
 C       2.847310     0.907389    -2.911228      57.35
 H       2.753578     0.523281    -3.862144      25.60
 C       2.527757     2.503983    -1.065393      75.59
 C       1.988092     3.778891    -0.503524      89.69
 H       2.242871     4.633577    -1.254574      24.14
 O       2.417937     4.225554     0.928688     206.83
 H       3.347198     4.729571     0.970672      29.43
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 C       0.282911     3.603074    -0.341084      48.18
 H       0.004565     3.627231    -1.452993      20.24
 C      -0.443562     5.158971     0.090712      87.54
 O       0.248457     6.231609    -0.717350     139.88
 H       0.317501     6.050746    -1.792432      25.70
 H      -0.264369     5.681660     0.992822      25.25
 H      -1.509277     5.121376    -0.131180      25.58
 C      -1.049817    -1.103773    -0.034702     -13.07
 H      -0.601644    -2.011505     0.231871      22.54
 C      -2.886864     0.490778    -0.921694      65.17
 H      -3.957700     0.464253    -1.169035      22.20
 C      -1.959389     1.493701    -0.534170     -13.77
 O      -2.517491     2.976598    -0.656728      91.91
 C      -4.033834     3.107039    -0.793624     116.84
 H      -4.436534     2.366624    -0.155802      27.32
 H      -4.009363     4.073991    -0.454459      27.19
 H      -4.265590     2.947252    -1.798706      27.64
 C      -0.637619     1.380201     0.024987      23.57
 O       0.017239     2.514317     0.504335     172.86
 C      -0.142338     0.109304     0.225985      -5.21
 H       1.063819     0.092638     0.660661      19.32
 C      -2.423097    -0.744390    -0.625538       0.08
 C      -3.260953    -2.082462    -0.997101      74.91
 H      -3.889896    -2.030718    -1.892659      20.67
 O      -2.202917    -3.192426    -1.495895     157.61
 H      -2.633161    -4.169469    -1.687725      17.09
 C      -4.139476    -2.789325     0.008067      81.61
 H      -3.485682    -3.129855     1.037067      17.91
 O      -5.014464    -1.729702     0.767891     241.26
 H      -5.152658    -2.375763     1.606155      25.11
 C      -5.066296    -3.807905    -0.563566      87.08
 O      -4.388615    -4.873777    -1.475194     237.76
 H      -3.726765    -5.519041    -0.946374      25.85
 H      -5.753378    -3.311435    -1.245821      27.03
 H      -5.234119    -4.498499     0.357173      25.63
55
name = lig-etoh-frame_804
 C       2.280768     2.217881    -2.458960      53.99
 H       1.489393     2.655539    -3.091886      21.35
 C       3.449980     1.728222    -0.221320      47.32
 H       3.739815     1.863330     0.802984      18.12
 C       3.823477     0.423189    -0.612089      20.14
 O       4.645515    -0.353588     0.144875     231.24
 C       4.854050    -0.106914     1.502498     118.49
 H       3.840810     0.210760     2.022758      24.71
 H       5.380792     0.912947     1.658758      26.40
 H       5.442439    -0.865755     1.956655      27.27
 C       3.470777     0.024067    -1.968666      20.65
 O       3.890040    -1.314016    -2.330022     210.27
 H       4.630474    -1.650788    -1.979497      27.29
 C       2.937415     0.977506    -2.920035      44.94
 H       2.610493     0.690972    -4.027394      23.13
 C       2.503089     2.549685    -1.023219      39.55
 C       1.962053     3.791022    -0.470364     108.06
 H       2.325938     4.656653    -1.198020      23.27
 O       2.482477     4.167911     0.901370     240.69
 H       3.361155     4.432468     0.733487      32.57
 C       0.271252     3.630706    -0.338005      63.71
 H       0.004054     3.447274    -1.346911      22.86
 C      -0.424517     5.170218     0.054505      89.11
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 O       0.243865     6.253763    -0.726154     177.91
 H       0.218337     6.193938    -1.643162      30.35
 H      -0.054240     5.498758     1.110671      24.77
 H      -1.539844     5.313201    -0.092143      25.70
 C      -1.083335    -1.000284    -0.048517      -5.48
 H      -0.861834    -2.158992     0.153388      20.86
 C      -2.901128     0.519379    -0.881883      40.20
 H      -3.881569     0.913699    -1.232366      21.48
 C      -2.004673     1.583869    -0.578726     -10.66
 O      -2.540045     2.945781    -0.680008     123.08
 C      -4.046827     3.091727    -0.788452      69.62
 H      -4.396942     2.183377    -0.177138      22.75
 H      -4.049864     4.324873    -0.591704      22.02
 H      -4.422895     2.945000    -2.114866      21.91
 C      -0.616313     1.370446     0.024158     -15.15
 O       0.001688     2.499708     0.437982     164.48
 C      -0.094091     0.067057     0.273028      83.10
 H       0.902392     0.101898     0.146054      23.75
 C      -2.452025    -0.883429    -0.635434       9.81
 C      -3.244999    -2.149988    -0.998545      86.83
 H      -3.750460    -1.824254    -1.965485      20.67
 O      -2.184050    -3.202641    -1.517354     219.79
 H      -2.767214    -3.905616    -1.645786      22.72
 C      -4.027690    -2.791837     0.020025     107.89
 H      -3.430908    -3.075859     0.779097      23.96
 O      -5.019167    -1.695911     0.746189     264.12
 H      -5.067302    -2.113983     1.543188      28.36
 C      -5.032982    -3.847726    -0.582470      97.48
 O      -4.395565    -4.860163    -1.460255     319.70
 H      -3.782774    -5.392527    -1.006822      31.05
 H      -5.866168    -3.236523    -1.035307      26.72
 H      -5.476495    -4.396811     0.206343      28.52
55
name = lig-etoh-frame_805
 C       2.279298     2.169118    -2.395387      64.58
 H       1.647438     2.683568    -3.130095      23.15
 C       3.405266     1.748321    -0.233774      55.83
 H       3.850808     1.970815     0.755925      19.79
 C       3.838234     0.480539    -0.585536      21.04
 O       4.665893    -0.359058     0.115138     234.27
 C       4.904381    -0.054454     1.542114     111.14
 H       3.873133     0.013592     1.819815      25.36
 H       5.463461     0.870055     1.683786      27.20
 H       5.463589    -1.038573     1.776113      25.25
 C       3.529294     0.043693    -1.907863       3.24
 O       3.866988    -1.356952    -2.395596     130.22
 H       4.605048    -1.850863    -1.648894      18.72
 C       2.978463     1.042293    -2.908274      40.70
 H       2.666923     0.790685    -3.934584      23.57
 C       2.531743     2.543647    -1.016395      12.67
 C       1.899217     3.843040    -0.386665     108.16
 H       2.135595     4.706034    -1.107835      20.07
 O       2.523451     4.099693     0.847143     264.70
 H       3.551955     4.094879     0.642053      26.22
 C       0.302656     3.745209    -0.383790      56.42
 H      -0.119685     3.277743    -1.364988      20.09
 C      -0.352116     5.174105     0.020519     115.35
 O       0.234826     6.262503    -0.715064     178.94
 H       0.022686     6.092998    -1.745723      24.81
 H      -0.075196     5.094901     1.053162      25.33
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 H      -1.416234     5.219203    -0.036200      26.10
 C      -1.135104    -0.924881    -0.077376      26.18
 H      -0.959836    -1.918910     0.004300      24.45
 C      -2.877292     0.527004    -0.832703      22.36
 H      -3.719155     0.971480    -1.355695      20.61
 C      -2.058708     1.668575    -0.598094       7.39
 O      -2.552675     2.892457    -0.704025     227.61
 C      -4.006724     3.085807    -0.839435     131.36
 H      -4.612888     2.488291    -0.171977      27.82
 H      -4.374915     4.000455    -0.608782      28.93
 H      -4.447281     2.970158    -1.722897      29.02
 C      -0.692484     1.371014    -0.015711     -22.33
 O       0.007980     2.495322     0.416793      94.07
 C      -0.141022     0.032937     0.265989      78.77
 H       1.019705    -0.172896    -0.086942      21.33
 C      -2.414847    -0.968007    -0.610554      24.31
 C      -3.150076    -2.168677    -1.081918      97.89
 H      -3.752044    -1.752440    -1.872340      22.43
 O      -2.181090    -3.179623    -1.524655     223.48
 H      -2.948900    -3.881503    -1.742017      17.68
 C      -4.021884    -2.765483     0.065888      64.82
 H      -3.092789    -3.326377     0.811149      19.44
 O      -4.991405    -1.697632     0.685810     248.04
 H      -4.984177    -1.835457     1.802565      23.44
 C      -4.987732    -3.893472    -0.563526     102.46
 O      -4.412280    -4.833683    -1.457110     271.58
 H      -3.794096    -5.362315    -0.825377      27.05
 H      -5.845119    -3.328102    -1.023049      26.27
 H      -5.801320    -4.324096     0.205130      26.75
55
name = lig-etoh-frame_806
 C       2.313610     2.111953    -2.304759      71.48
 H       1.863347     2.866928    -3.029639      24.54
 C       3.363046     1.773954    -0.213393      55.64
 H       3.710337     2.370248     0.654882      19.27
 C       3.852728     0.522801    -0.627173      15.53
 O       4.699355    -0.366710     0.082231     210.58
 C       4.944516    -0.033521     1.543278     111.74
 H       3.902573    -0.195703     2.097610      24.76
 H       5.572132     0.844278     1.738036      26.05
 H       5.391922    -0.947218     1.848883      27.04
 C       3.590715     0.037836    -1.924570       8.38
 O       3.848159    -1.357004    -2.425939     192.50
 H       4.316904    -1.704922    -1.651536      23.66
 C       2.999085     1.043808    -2.834708      48.28
 H       2.866737     0.712796    -3.901339      22.33
 C       2.546470     2.550082    -1.028090      20.64
 C       1.845755     3.871793    -0.354069      95.96
 H       1.902766     4.815691    -1.102072      18.21
 O       2.558857     4.044522     0.806363     321.25
 H       3.542869     3.808975     0.821479      24.18
 C       0.336898     3.823818    -0.469065      68.29
 H       0.022751     3.573383    -1.431269      21.90
 C      -0.266036     5.120332     0.000839     115.77
 O       0.219023     6.256406    -0.716914     183.17
 H      -0.059646     5.981055    -1.661141      27.64
 H      -0.062882     5.098383     1.123611      23.86
 H      -1.405341     4.985042    -0.051861      23.84
 C      -1.163555    -0.930703    -0.101224      15.38
 H      -0.590447    -2.011100    -0.032445      21.93
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 C      -2.836173     0.491569    -0.807205      45.60
 H      -3.762303     0.540693    -1.453593      18.87
 C      -2.076691     1.619210    -0.567954      23.51
 O      -2.583455     2.894256    -0.731620     222.71
 C      -3.968165     3.066246    -0.841116      96.56
 H      -4.686696     2.593995    -0.074051      25.08
 H      -4.443495     4.156831    -0.473521      23.46
 H      -4.502735     2.783728    -2.086196      22.10
 C      -0.782364     1.409696    -0.056148      -6.66
 O       0.026355     2.506643     0.433792      43.75
 C      -0.231030     0.064396     0.181638      67.31
 H       0.716380    -0.379473     0.162270      24.87
 C      -2.386546    -0.870433    -0.593564      38.63
 C      -3.051324    -2.144323    -1.145789      83.66
 H      -3.872237    -1.864390    -1.903010      22.78
 O      -2.211265    -3.161760    -1.537338     265.28
 H      -2.735248    -3.944320    -1.962678      19.02
 C      -4.039571    -2.769551     0.131510      87.17
 H      -3.362479    -3.221531     0.713694      26.24
 O      -4.928477    -1.741531     0.637121     367.28
 H      -4.735692    -1.609995     1.591335      30.04
 C      -5.012019    -3.885761    -0.496104      97.58
 O      -4.407520    -4.824133    -1.436434     270.85
 H      -3.847006    -5.436115    -0.815504      27.37
 H      -5.606175    -3.344627    -1.283941      26.10
 H      -5.596100    -4.367344     0.223443      28.02
55
name = lig-etoh-frame_807
 C       2.352577     2.108105    -2.272042      72.75
 H       2.005629     2.877349    -2.892841      25.81
 C       3.341184     1.804979    -0.179123      43.27
 H       3.623777     2.295689     0.701656      21.34
 C       3.891104     0.534437    -0.670399      14.85
 O       4.731862    -0.350456     0.078192     210.12
 C       4.942552    -0.067956     1.526783     114.50
 H       4.176058    -0.005998     2.260770      27.02
 H       5.538681     0.893647     1.743896      25.95
 H       5.583542    -0.908146     1.990797      26.05
 C       3.621493     0.031136    -2.002428      23.05
 O       3.814529    -1.290514    -2.431482     172.43
 H       4.305391    -1.725860    -1.661972      22.69
 C       3.013235     0.950050    -2.755083      61.20
 H       3.112368     0.683069    -3.893969      21.56
 C       2.524556     2.589217    -1.008054      34.45
 C       1.867566     3.857065    -0.427307     104.21
 H       2.032913     4.833837    -1.104028      18.07
 O       2.555456     4.021514     0.823391     345.59
 H       3.469539     3.863993     0.831197      29.37
 C       0.393999     3.830489    -0.511781      57.32
 H       0.212948     3.823341    -1.675459      18.28
 C      -0.234854     5.038558     0.043079     116.29
 O       0.187908     6.229103    -0.727916     165.77
 H       0.052134     6.092452    -1.668235      31.72
 H       0.009414     5.412045     1.037377      24.12
 H      -1.271414     4.872271    -0.119803      24.72
 C      -1.078612    -1.034211    -0.093268      50.61
 H      -0.520264    -1.863394    -0.076778      25.06
 C      -2.853104     0.412017    -0.835822      72.01
 H      -3.778508     0.221661    -1.339550      21.92
 C      -2.101511     1.541631    -0.517747      13.22
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 O      -2.606892     2.919945    -0.753420     193.09
 C      -4.037347     3.072930    -0.862609     125.14
 H      -4.419878     2.362225    -0.128123      27.16
 H      -3.969129     4.094983    -0.728126      26.40
 H      -4.184343     2.763628    -1.770431      29.18
 C      -0.795589     1.476048    -0.054818      24.67
 O       0.025177     2.529919     0.438379      73.06
 C      -0.375918     0.146486     0.072353       4.56
 H       0.695195    -0.188553     0.551173      21.06
 C      -2.399065    -0.760084    -0.623528      25.03
 C      -3.061563    -2.093120    -1.144270      70.34
 H      -3.771201    -1.974306    -1.934020      22.58
 O      -2.201520    -3.159409    -1.574118     296.19
 H      -2.631667    -3.842476    -1.979143      26.02
 C      -4.080353    -2.768511     0.111231      70.28
 H      -3.371020    -3.225573     1.125340      19.72
 O      -4.851821    -1.785483     0.585916     365.50
 H      -4.537824    -1.607175     1.461321      29.29
 C      -5.033341    -3.824281    -0.463130      79.73
 O      -4.377296    -4.846491    -1.391533     300.49
 H      -3.872147    -5.510239    -0.995776      30.99
 H      -5.549676    -3.271952    -1.297445      25.76
 H      -5.513214    -4.465844     0.383256      24.26
55
name = lig-etoh-frame_808
 C       2.407904     2.123346    -2.296081      58.54
 H       1.966250     2.831167    -3.113725      21.27
 C       3.355050     1.782878    -0.161293      61.02
 H       3.648354     1.878951     0.959699      19.24
 C       3.931678     0.548339    -0.679240      35.78
 O       4.749831    -0.320759     0.105368     224.18
 C       4.980688    -0.105591     1.517946     126.68
 H       4.075824     0.199407     2.225147      25.10
 H       5.459840     0.863002     1.546619      29.68
 H       5.733890    -0.795931     1.862112      27.49
 C       3.655676     0.006973    -1.994038      30.13
 O       3.787314    -1.209610    -2.423291     105.58
 H       4.490364    -1.840401    -1.799542      21.39
 C       2.985738     0.889495    -2.771352      62.85
 H       3.064643     0.747469    -3.798181      24.26
 C       2.506798     2.602994    -0.966438      50.67
 C       1.981624     3.832040    -0.527723     123.97
 H       2.412837     4.736732    -1.101939      20.05
 O       2.496477     4.032199     0.874272     268.76
 H       3.543675     4.157891     0.694067      25.45
 C       0.472562     3.780836    -0.521897      62.43
 H       0.213554     3.743428    -1.560189      19.97
 C      -0.237147     5.007612     0.081742      99.56
 O       0.148253     6.192490    -0.738811     152.29
 H       0.209756     6.145292    -1.817790      26.87
 H       0.075265     5.447526     1.044990      22.86
 H      -1.356957     4.850493    -0.039578      22.95
 C      -1.022832    -1.071541    -0.110701      57.20
 H      -0.493514    -2.150091    -0.066762      20.48
 C      -2.936246     0.406546    -0.892777      49.26
 H      -3.982850     0.439736    -1.280833      22.04
 C      -2.164689     1.574885    -0.491859      -2.96
 O      -2.580770     2.899958    -0.758558     155.08
 C      -4.061292     3.067079    -0.849194      86.15
 H      -4.450828     2.327618    -0.112879      24.84
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 H      -3.964742     4.259146    -0.935830      21.82
 H      -4.336824     2.649576    -2.120391      21.93
 C      -0.793654     1.542522    -0.038464       7.24
 O       0.006109     2.566698     0.407913     125.55
 C      -0.409514     0.197434     0.026191      22.35
 H       0.375992     0.484384     0.737740      21.40
 C      -2.329084    -0.884094    -0.655081       6.40
 C      -3.137802    -2.077547    -1.087127      73.82
 H      -3.764293    -1.837511    -2.021410      19.65
 O      -2.139701    -3.131250    -1.605950     196.67
 H      -2.892077    -3.863772    -1.966043      15.43
 C      -4.027323    -2.807435     0.073605     116.62
 H      -3.516698    -3.149287     0.833835      24.81
 O      -4.817847    -1.778226     0.553890     362.04
 H      -4.422467    -1.602981     1.572789      25.57
 C      -5.015614    -3.802441    -0.460488      93.94
 O      -4.353550    -4.862965    -1.352497     287.62
 H      -3.765998    -5.612944    -0.898786      25.86
 H      -5.826832    -3.268088    -0.997675      27.39
 H      -5.585440    -4.271560     0.344752      26.89
55
name = lig-etoh-frame_809
 C       2.466087     2.148487    -2.361013      51.08
 H       1.965491     2.616537    -3.140313      20.24
 C       3.401720     1.703793    -0.134279      63.87
 H       3.466572     1.659402     0.912607      19.96
 C       3.969137     0.554384    -0.652048      26.79
 O       4.750131    -0.306034     0.127702     249.64
 C       5.018929    -0.072539     1.507077     116.45
 H       4.069374    -0.025058     1.969859      27.31
 H       5.564973     0.948630     1.434599      26.08
 H       5.739095    -0.878450     1.792810      26.21
 C       3.673778     0.041861    -1.895722      30.01
 O       3.803364    -1.213110    -2.420034     215.66
 H       4.498465    -1.618601    -2.061424      29.59
 C       2.921599     0.912279    -2.817338      46.46
 H       2.800829     0.707564    -4.027754      22.49
 C       2.560064     2.509864    -0.970016      60.89
 C       2.108367     3.852109    -0.546584     121.70
 H       2.577461     4.673392    -1.230932      26.31
 O       2.444487     4.059787     0.910896     278.21
 H       3.317608     4.514272     0.831217      30.90
 C       0.522710     3.732512    -0.488381      73.63
 H       0.024578     3.446996    -1.492398      21.57
 C      -0.246752     5.012609     0.072309     106.89
 O       0.113108     6.162704    -0.762325     239.14
 H       0.211825     5.854752    -1.660757      31.92
 H       0.108486     5.141541     1.129674      25.05
 H      -1.312496     4.841610     0.184362      25.30
 C      -0.988319    -1.065393    -0.161996      76.69
 H      -0.654825    -2.062583     0.049802      22.75
 C      -2.981221     0.422285    -0.917343      35.45
 H      -3.992564     0.743174    -1.190689      21.34
 C      -2.231930     1.648751    -0.506667       2.88
 O      -2.570592     2.865685    -0.754110     208.78
 C      -4.033847     3.061647    -0.928254     141.68
 H      -4.708600     2.683166    -0.101454      28.20
 H      -4.456646     4.041043    -0.874365      27.70
 H      -4.527060     2.766664    -1.709738      30.53
 C      -0.872179     1.561318    -0.070842       4.62
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 O      -0.006246     2.619959     0.363168     154.68
 C      -0.350695     0.260932     0.071795      27.40
 H       0.507273     0.529466     0.776937      20.32
 C      -2.271945    -1.038041    -0.692092      -8.53
 C      -3.193446    -2.123846    -1.048729      94.85
 H      -3.775857    -1.678136    -1.832698      21.03
 O      -2.115628    -3.103897    -1.638846     230.11
 H      -2.784847    -3.779290    -1.762604      18.91
 C      -3.965620    -2.812570    -0.030978      81.92
 H      -3.117908    -3.413958     0.809515      17.12
 O      -4.806953    -1.726122     0.572159     368.11
 H      -4.596269    -1.654404     1.485457      30.02
 C      -4.993121    -3.827866    -0.480941      93.00
 O      -4.342773    -4.875944    -1.317427     328.77
 H      -3.780977    -5.366285    -0.643692      29.20
 H      -5.965169    -3.374945    -0.851912      26.53
 H      -5.575798    -4.215902     0.440153      26.80
55
name = lig-etoh-frame_810
 C       2.518643     2.156657    -2.412011      59.95
 H       1.829767     2.784334    -3.113674      19.61
 C       3.418446     1.633455    -0.121674      67.30
 H       3.275719     1.855710     0.987515      17.18
 C       4.023586     0.515251    -0.595632      18.37
 O       4.754395    -0.324868     0.121126     244.15
 C       5.077824     0.001062     1.466961     118.09
 H       4.078949    -0.257376     2.046304      24.54
 H       5.581703     0.903750     1.688804      27.60
 H       5.596492    -0.928737     1.830938      25.57
 C       3.625275     0.118896    -1.889475      15.11
 O       3.826469    -1.237496    -2.419534     117.41
 H       4.829631    -1.626823    -2.071622      22.13
 C       2.885330     0.922310    -2.860642      46.16
 H       2.614627     0.575163    -3.753300      27.08
 C       2.674142     2.395546    -1.007130      78.34
 C       2.179648     3.856946    -0.488755     107.22
 H       2.503619     4.616478    -1.330431      28.17
 O       2.401686     4.108695     0.920639     297.58
 H       3.137322     4.693979     1.166993      32.16
 C       0.499053     3.707779    -0.482920      79.49
 H       0.082908     3.330253    -1.435875      21.72
 C      -0.217899     5.000789     0.060987     112.23
 O       0.074718     6.123234    -0.770072     247.29
 H       0.152262     5.616081    -1.649283      28.95
 H       0.191597     4.980778     1.074143      25.17
 H      -1.315402     4.817297     0.212004      24.74
 C      -0.967448    -0.987379    -0.211580      22.67
 H      -0.542684    -1.976122     0.192649      22.22
 C      -2.931344     0.432299    -0.886947      38.05
 H      -3.963974     0.629000    -1.183138      22.05
 C      -2.266932     1.605723    -0.550160      15.84
 O      -2.641036     2.910415    -0.764265     228.63
 C      -4.041359     3.083211    -0.948771     119.18
 H      -4.636958     2.829022    -0.052187      26.73
 H      -4.508835     4.141508    -0.839279      24.78
 H      -4.674838     2.516782    -1.965929      23.51
 C      -0.934723     1.534297    -0.117173       6.02
 O      -0.017785     2.661261     0.342094     139.49
 C      -0.270666     0.311018     0.167513      28.38
 H       0.785324     0.033044     0.544993      21.47
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 C      -2.285873    -1.024981    -0.718525       1.00
 C      -3.152153    -2.175734    -1.079843      92.21
 H      -3.931364    -1.714319    -1.774938      21.11
 O      -2.138954    -3.075728    -1.656798     233.85
 H      -2.561281    -4.016441    -1.771217      17.49
 C      -3.924841    -2.825080    -0.046786     103.07
 H      -3.204345    -3.288702     0.453470      22.89
 O      -4.791822    -1.686343     0.590460     336.10
 H      -4.692676    -1.780721     1.591169      27.52
 C      -5.002895    -3.875338    -0.481523      89.41
 O      -4.346758    -4.881612    -1.265183     359.70
 H      -3.766760    -5.223298    -0.601133      31.25
 H      -5.775153    -3.452144    -1.102282      27.68
 H      -5.222954    -4.316953     0.523365      27.44
55
name = lig-etoh-frame_811
 C       2.528614     2.194615    -2.440477      55.07
 H       1.931330     2.964023    -2.838168      20.04
 C       3.399108     1.603727    -0.076864      67.76
 H       3.301799     2.146696     0.874445      21.11
 C       4.045411     0.460801    -0.581711       7.99
 O       4.799110    -0.378100     0.114476     217.49
 C       5.092368     0.005501     1.466270     126.66
 H       4.291119    -0.062030     2.155253      27.08
 H       5.529670     0.985144     1.886274      25.66
 H       5.693315    -0.820118     1.817754      27.13
 C       3.572217     0.133849    -1.967871      18.66
 O       3.879295    -1.250428    -2.396834     152.20
 H       4.779573    -1.541302    -2.058315      24.26
 C       2.892099     0.900983    -2.846843      58.24
 H       2.422707     0.230210    -3.781487      23.39
 C       2.785031     2.387841    -1.052446      34.43
 C       2.176288     3.795283    -0.425267      90.05
 H       2.424133     4.622642    -1.157179      23.58
 O       2.363146     4.161257     0.921728     292.37
 H       3.105215     4.747822     1.384627      27.49
 C       0.453558     3.697205    -0.514633      60.66
 H       0.282704     3.534893    -1.629780      18.69
 C      -0.181053     4.945296     0.062069     105.98
 O       0.041730     6.073348    -0.780546     219.99
 H       0.085328     5.761437    -1.806068      26.81
 H       0.323404     5.173732     1.049103      23.18
 H      -1.269034     4.790484     0.084758      23.58
 C      -0.955888    -0.877990    -0.230090      13.45
 H      -0.361213    -1.761001     0.172496      21.89
 C      -2.870536     0.374915    -0.847653      58.55
 H      -3.901469     0.246157    -1.230897      21.50
 C      -2.254954     1.552765    -0.600579       5.32
 O      -2.742458     2.977855    -0.785479     194.18
 C      -4.151257     3.117602    -0.970762     110.54
 H      -4.449265     2.586334    -0.009855      24.94
 H      -4.034979     4.216006    -1.146994      24.09
 H      -4.290998     2.543120    -1.771638      28.39
 C      -0.871320     1.502010    -0.115140      -2.01
 O      -0.050563     2.661733     0.354217     146.70
 C      -0.228936     0.278250     0.224985      35.72
 H       0.789373    -0.022050     0.271369      22.74
 C      -2.316159    -0.860387    -0.723142      24.70
 C      -3.084152    -2.187493    -1.186815      84.96
 H      -3.893059    -1.963114    -1.896922      21.78
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 O      -2.188266    -3.068998    -1.675490     270.10
 H      -2.258247    -4.110768    -1.802963      18.26
 C      -3.979722    -2.802565    -0.026934      53.77
 H      -3.066226    -3.365921     0.765798      18.40
 O      -4.746289    -1.673442     0.613987     284.39
 H      -4.805535    -2.061279     1.648366      22.97
 C      -4.978086    -3.904795    -0.458038      85.57
 O      -4.348811    -4.905207    -1.219533     329.07
 H      -3.541512    -5.414061    -0.709800      25.98
 H      -5.690030    -3.476975    -1.243896      25.92
 H      -5.258380    -4.390458     0.491815      27.03
55
name = lig-etoh-frame_812
 C       2.539595     2.228516    -2.408053      69.45
 H       2.016568     3.102380    -2.905335      21.29
 C       3.386822     1.594704    -0.057107      72.44
 H       3.560281     2.136787     0.891211      22.44
 C       3.989574     0.443745    -0.624455       1.97
 O       4.867506    -0.443619     0.120667     186.19
 C       5.114111    -0.015480     1.522665     104.96
 H       4.161419     0.090540     2.198658      24.25
 H       5.474159     1.025090     1.495566      25.92
 H       5.994636    -0.686813     1.834061      25.28
 C       3.600631     0.043884    -1.994331      11.78
 O       3.919588    -1.236714    -2.373963     182.99
 H       4.752854    -1.524974    -1.914336      22.92
 C       2.858766     0.863266    -2.878917      60.64
 H       2.495962     0.311574    -3.617571      26.89
 C       2.856053     2.488312    -1.070488      46.88
 C       2.119365     3.710482    -0.396369     101.37
 H       2.384501     4.739003    -0.966597      20.95
 O       2.323626     4.202762     0.959324     281.68
 H       3.225876     4.558818     1.076474      29.05
 C       0.452905     3.678123    -0.553270      57.32
 H       0.356185     3.761008    -1.669583      17.77
 C      -0.148540     4.897542     0.051938     105.95
 O       0.020930     6.045487    -0.819383     240.53
 H      -0.012371     5.953872    -1.731195      33.39
 H       0.261467     5.317478     0.949960      23.70
 H      -1.227737     4.689160     0.135407      23.52
 C      -0.954470    -0.795748    -0.215814      50.77
 H      -0.419222    -1.741246    -0.111727      23.81
 C      -2.905832     0.334823    -0.848823      52.87
 H      -3.874617     0.155116    -1.273336      20.55
 C      -2.174395     1.611123    -0.625667     -19.45
 O      -2.776406     2.982971    -0.796826     165.82
 C      -4.218282     3.153296    -0.958429      95.64
 H      -4.732451     2.663840    -0.120902      25.70
 H      -4.113368     4.165883    -1.365973      23.83
 H      -4.393006     2.446698    -2.023805      22.72
 C      -0.763733     1.507172    -0.078882      -3.45
 O      -0.103298     2.625521     0.359971     165.33
 C      -0.245993     0.230148     0.211176      64.29
 H       0.947510     0.300790     0.223854      22.94
 C      -2.268953    -0.781325    -0.710426      33.06
 C      -3.082547    -2.161942    -1.248793      71.41
 H      -3.737130    -2.005711    -2.169191      20.97
 O      -2.168652    -3.091996    -1.714992     297.70
 H      -2.441928    -3.965114    -1.680989      22.23
 C      -3.999496    -2.765375     0.035427      99.41
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 H      -3.425819    -3.148335     0.806378      24.05
 O      -4.684877    -1.705532     0.657963     364.18
 H      -4.863389    -2.047816     1.462433      29.27
 C      -4.925472    -3.917549    -0.422518      96.32
 O      -4.317667    -4.974145    -1.194888     363.33
 H      -3.580577    -5.485273    -0.905504      30.18
 H      -5.722840    -3.510397    -1.008148      27.37
 H      -5.710010    -4.308136     0.383421      26.49
55
name = lig-etoh-frame_813
 C       2.559605     2.227692    -2.369684      71.84
 H       2.181834     2.913001    -3.148926      22.90
 C       3.403515     1.608138    -0.099823      60.09
 H       3.856153     1.832883     0.921577      20.87
 C       3.923713     0.421569    -0.650804      -0.33
 O       4.907646    -0.495247     0.123091     209.74
 C       5.149263    -0.012467     1.561509     114.78
 H       4.222412    -0.042433     2.076639      26.87
 H       5.473273     0.985034     1.136700      24.58
 H       5.988362    -0.496654     1.962431      27.98
 C       3.644773    -0.038551    -1.969454      10.28
 O       3.963883    -1.235109    -2.370624     120.85
 H       4.706357    -1.668425    -1.607689      17.07
 C       2.835337     0.867781    -2.855062      31.02
 H       2.435644     0.414066    -3.949707      20.77
 C       2.878092     2.617076    -1.013533      61.24
 C       2.027946     3.694208    -0.396820     118.26
 H       2.276923     4.601889    -1.004610      22.80
 O       2.305350     4.213695     1.005937     279.14
 H       3.287607     4.293096     0.809478      27.93
 C       0.522554     3.652487    -0.556115      58.38
 H       0.145786     3.538752    -1.572811      21.83
 C      -0.150611     4.894989     0.008650      97.43
 O       0.010749     6.050872    -0.841304     210.37
 H      -0.170115     5.838429    -1.908010      25.28
 H       0.235429     5.227423     1.023122      23.44
 H      -1.200981     4.584828     0.273482      23.22
 C      -0.955934    -0.846503    -0.199634      74.80
 H      -0.555710    -1.913785    -0.534320      20.92
 C      -2.972905     0.448533    -0.874307      24.70
 H      -4.000415     0.469007    -1.314388      14.53
 C      -2.104581     1.682907    -0.628426     -10.69
 O      -2.758217     2.941237    -0.787569     179.59
 C      -4.242938     3.122966    -1.029293     115.53
 H      -5.122851     3.037478    -0.253064      25.52
 H      -4.642570     4.193280    -1.295884      25.45
 H      -4.739925     2.667861    -1.802877      26.85
 C      -0.750166     1.536479    -0.061629      19.37
 O      -0.136239     2.599390     0.353174     178.09
 C      -0.198337     0.284947     0.166181      81.49
 H       0.773281     0.398439     0.439709      23.87
 C      -2.201946    -0.858344    -0.711462       2.68
 C      -3.105778    -2.107567    -1.243727      68.09
 H      -3.613817    -1.746441    -2.152501      21.06
 O      -2.113900    -3.127576    -1.744383     226.26
 H      -2.801462    -3.938188    -1.572951      13.62
 C      -3.997262    -2.727407     0.046622      61.39
 H      -3.233213    -3.164540     1.009728      17.30
 O      -4.645167    -1.717257     0.681282     279.70
 H      -4.941159    -2.016703     1.700287      24.21
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 C      -4.918522    -3.932120    -0.373218      87.77
 O      -4.298345    -5.044453    -1.197422     327.93
 H      -3.521864    -5.572876    -0.738581      25.98
 H      -5.706728    -3.441565    -1.062335      26.02
 H      -5.669113    -4.238152     0.339523      27.50
55
name = lig-etoh-frame_814
 C       2.603125     2.177197    -2.345752      47.11
 H       2.235110     2.748671    -3.185883      22.07
 C       3.467801     1.631989    -0.169211      50.24
 H       3.790357     1.695940     0.817151      21.34
 C       3.896731     0.371734    -0.640153       8.89
 O       4.905368    -0.537262     0.115273     192.31
 C       5.187579     0.018036     1.508980     103.70
 H       4.256935    -0.137057     2.145089      25.96
 H       5.494155     1.093794     1.347611      25.61
 H       6.008625    -0.522666     2.145136      26.21
 C       3.623157    -0.036757    -1.948682      18.04
 O       4.039888    -1.293681    -2.363563     195.20
 H       4.479583    -1.687229    -1.709823      26.15
 C       2.836064     0.867018    -2.799808      55.20
 H       2.648644     0.826130    -3.815086      24.00
 C       2.861066     2.678212    -0.929800      60.34
 C       1.945346     3.750083    -0.397448     103.38
 H       2.123570     4.602262    -1.248700      22.89
 O       2.310927     4.195547     1.018642     265.95
 H       3.379136     4.107150     0.986055      25.41
 C       0.547545     3.610279    -0.534070      70.27
 H       0.036844     3.150836    -1.449050      21.23
 C      -0.171293     4.918033    -0.016252     107.86
 O      -0.003313     6.058968    -0.880900     259.81
 H      -0.201673     5.642327    -1.723058      30.44
 H       0.296507     5.051644     0.935620      25.17
 H      -1.192406     4.624668     0.165981      24.57
 C      -0.915350    -0.982116    -0.215578      28.57
 H      -0.468621    -1.869753    -0.493487      20.89
 C      -2.932239     0.575363    -0.886409      32.95
 H      -3.921387     0.858694    -1.233843      18.24
 C      -2.142219     1.676216    -0.636142      15.69
 O      -2.752331     2.917961    -0.773954     152.66
 C      -4.309259     3.123043    -1.084836     100.88
 H      -4.926495     3.135943    -0.184513      26.06
 H      -4.530393     4.173795    -1.203855      26.06
 H      -4.891281     2.482465    -1.950343      23.15
 C      -0.830400     1.548269    -0.085484      28.01
 O      -0.114245     2.632039     0.374249     148.44
 C      -0.167186     0.343665     0.097196      15.34
 H       0.840847     0.247804     0.781596      20.14
 C      -2.274207    -0.875725    -0.748713     -13.94
 C      -3.064998    -2.037985    -1.183936      77.40
 H      -3.702782    -1.548865    -1.960590      20.94
 O      -2.116157    -3.174262    -1.732233     200.22
 H      -2.838695    -3.923330    -1.751077      15.88
 C      -3.920372    -2.745467     0.060670      72.15
 H      -3.054608    -3.155358     0.603624      21.06
 O      -4.655715    -1.694373     0.718887     342.62
 H      -4.719663    -1.963519     1.699545      26.58
 C      -4.935987    -3.924074    -0.378560      80.04
 O      -4.282304    -5.097878    -1.188277     286.07
 H      -3.632507    -5.521752    -0.512529      26.13
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 H      -5.458310    -3.486424    -1.189539      26.81
 H      -5.399235    -4.384709     0.635914      25.74
55
name = lig-etoh-frame_815
 C       2.649531     2.145329    -2.283891      45.60
 H       2.138123     2.839601    -3.030303      21.76
 C       3.549839     1.658579    -0.220456      61.35
 H       3.556286     1.877218     0.941741      20.05
 C       3.915851     0.314345    -0.615053      18.14
 O       4.871526    -0.545155     0.116180     215.20
 C       5.216367     0.039408     1.449282     118.67
 H       4.365541    -0.052852     2.143729      28.40
 H       5.483732     1.109383     1.675388      26.68
 H       5.940930    -0.586292     1.893787      29.23
 C       3.579195    -0.049598    -1.941744      12.66
 O       4.084598    -1.334007    -2.393215     130.28
 H       4.618084    -1.863193    -1.530401      18.13
 C       2.888389     0.876409    -2.703112      68.51
 H       2.851139     0.861193    -3.883089      23.82
 C       2.816564     2.634665    -0.907683      55.21
 C       1.971055     3.844398    -0.406860      92.09
 H       2.024200     4.684812    -1.175257      22.95
 O       2.334432     4.160233     0.995539     344.87
 H       3.199061     4.110501     1.288232      31.16
 C       0.433235     3.549774    -0.507294      82.17
 H       0.334197     3.171498    -1.522051      21.84
 C      -0.190649     4.924779    -0.042811     100.96
 O      -0.015108     6.052833    -0.907937     233.45
 H      -0.134101     5.678993    -1.829663      27.71
 H       0.361920     5.099994     0.930948      23.30
 H      -1.317409     4.753103    -0.023548      22.53
 C      -0.903835    -1.023082    -0.265306     -40.54
 H      -0.167837    -2.013229    -0.207467      17.13
 C      -2.844196     0.585035    -0.896793      59.22
 H      -3.864240     0.878929    -1.156300      21.46
 C      -2.216667     1.674515    -0.633929      27.42
 O      -2.775566     2.930897    -0.770850     158.63
 C      -4.372305     3.127093    -1.118435      90.14
 H      -4.605230     2.804464    -0.019976      23.67
 H      -4.025256     4.202983    -1.433676      22.95
 H      -4.610140     2.404899    -1.900844      25.10
 C      -0.876820     1.562005    -0.106093       0.22
 O      -0.078131     2.672778     0.441292     164.19
 C      -0.173871     0.299225     0.037545      -3.89
 H       0.579059     0.229840     0.710822      22.81
 C      -2.328601    -0.792435    -0.761152       4.93
 C      -3.034695    -2.008476    -1.124973      87.59
 H      -3.871323    -1.719463    -1.814691      21.01
 O      -2.173726    -3.191501    -1.697707     208.75
 H      -2.672610    -3.987688    -1.942145      20.21
 C      -3.840046    -2.756284     0.033439      57.46
 H      -2.765191    -3.252230     0.424108      17.76
 O      -4.660665    -1.681041     0.756490     324.71
 H      -4.514715    -1.971976     1.709989      25.29
 C      -4.896902    -3.929013    -0.388376      92.89
 O      -4.283736    -5.114973    -1.146112     326.96
 H      -3.688094    -5.538811    -0.569899      31.37
 H      -5.617706    -3.520904    -1.172854      26.21
 H      -5.203599    -4.315548     0.499777      27.86
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name = lig-etoh-frame_816
 C       2.648233     2.193478    -2.204325      52.15
 H       2.128043     2.873549    -2.805359      22.34
 C       3.616889     1.679492    -0.171591      84.56
 H       3.501069     1.996093     0.799395      21.42
 C       3.955391     0.295985    -0.590053      16.51
 O       4.814458    -0.501999     0.126290     205.27
 C       5.222707     0.036125     1.409891     107.46
 H       4.341556    -0.047918     2.099311      26.78
 H       5.577191     1.123337     1.606181      25.44
 H       6.050317    -0.743638     1.587378      26.09
 C       3.584350    -0.137226    -1.897290       7.10
 O       4.094921    -1.350719    -2.416367     179.19
 H       4.770149    -1.689919    -1.781672      22.83
 C       2.965001     0.879020    -2.680331      57.31
 H       3.006677     0.553972    -3.747386      23.96
 C       2.765509     2.541220    -0.948722      50.31
 C       2.062458     3.882396    -0.395316      79.64
 H       2.118743     4.924830    -0.993723      20.47
 O       2.323225     4.131334     0.963349     295.93
 H       3.273919     4.156239     1.359607      27.37
 C       0.338479     3.548977    -0.487256      76.42
 H       0.442473     3.363589    -1.593936      18.99
 C      -0.241564     4.915216    -0.085749     107.78
 O      -0.014197     6.043099    -0.938282     240.03
 H       0.080496     5.922996    -2.010246      24.22
 H       0.161450     5.243954     0.862694      24.51
 H      -1.298548     4.845842     0.031581      24.87
 C      -0.900111    -0.963879    -0.329537      68.48
 H      -0.465512    -1.800379     0.006985      24.47
 C      -2.827513     0.456549    -0.930977      62.44
 H      -3.903591     0.430499    -1.183141      24.01
 C      -2.200825     1.770783    -0.592005       7.61
 O      -2.797192     2.952152    -0.777483     165.74
 C      -4.322377     3.131328    -1.108289     100.88
 H      -4.686088     2.688062    -0.172916      25.20
 H      -4.113225     4.036850    -1.569288      25.10
 H      -4.529590     2.393614    -1.956847      25.30
 C      -0.855039     1.560717    -0.098720       4.17
 O      -0.070591     2.662314     0.521546     179.93
 C      -0.283737     0.216438    -0.032035      13.01
 H       0.714447     0.294780     0.636142      20.02
 C      -2.269421    -0.720556    -0.745230      21.53
 C      -3.091285    -2.057383    -1.106111      93.43
 H      -3.878428    -1.957078    -1.848467      20.61
 O      -2.227836    -3.154702    -1.648662     221.13
 H      -2.723554    -4.033793    -2.088467      16.41
 C      -3.757475    -2.754159    -0.009436      84.59
 H      -2.977910    -3.246840     0.658078      19.90
 O      -4.635819    -1.708035     0.786535     279.83
 H      -4.356723    -1.974925     1.833517      22.36
 C      -4.794594    -3.923168    -0.440459      87.95
 O      -4.316874    -5.094827    -1.103840     300.77
 H      -3.517553    -5.644401    -0.657208      26.47
 H      -5.780402    -3.593038    -0.823834      26.19
 H      -5.353921    -4.266680     0.615938      25.46
55
name = lig-etoh-frame_817
 C       2.608927     2.198256    -2.239112      45.28
 H       2.070908     2.949757    -2.920979      19.91
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 C       3.638466     1.670702    -0.114024      78.41
 H       3.754642     2.000782     1.009020      18.51
 C       3.977404     0.352374    -0.563984      25.47
 O       4.756915    -0.443634     0.138784     215.57
 C       5.239419    -0.001122     1.394273     123.59
 H       4.414896    -0.134108     2.129446      26.21
 H       5.667079     1.003228     1.209436      26.89
 H       6.057997    -0.672923     1.583432      27.62
 C       3.614221    -0.200061    -1.836127       8.20
 O       4.067548    -1.334949    -2.454360     129.98
 H       5.027533    -1.677924    -1.943227      19.95
 C       3.061487     0.852519    -2.681156      40.73
 H       2.970509     0.449136    -3.717658      23.79
 C       2.755132     2.487942    -0.899801      34.69
 C       2.140307     3.865580    -0.378320      88.07
 H       2.362820     4.828733    -0.922226      22.91
 O       2.309748     4.105021     0.967223     269.61
 H       3.334477     4.276184     1.065589      27.05
 C       0.352399     3.637627    -0.467997      55.61
 H       0.058372     3.335224    -1.506940      20.09
 C      -0.320849     4.917737    -0.141013     104.45
 O       0.009112     6.058332    -0.983625     270.64
 H       0.185025     5.849704    -1.876988      30.67
 H       0.009318     5.289028     0.877128      23.21
 H      -1.441895     4.803523     0.113193      23.31
 C      -0.937785    -0.873410    -0.395612      88.84
 H      -0.746840    -1.945692     0.135612      21.12
 C      -2.860589     0.417160    -0.964407      42.73
 H      -3.854342     0.088872    -1.268093      20.89
 C      -2.163377     1.785353    -0.553984      -5.00
 O      -2.813393     2.992870    -0.784011     182.24
 C      -4.201058     3.072417    -1.112183     106.90
 H      -5.068867     2.919979    -0.287048      24.83
 H      -4.587564     4.205640    -1.494380      23.72
 H      -4.561413     2.414471    -2.015887      24.78
 C      -0.837219     1.559700    -0.076046      17.71
 O      -0.086136     2.601295     0.569865     148.81
 C      -0.341239     0.232584    -0.037158      60.57
 H       0.695195     0.237489     0.202154      22.93
 C      -2.187006    -0.801075    -0.752433       0.77
 C      -3.143107    -2.115453    -1.128352      80.81
 H      -3.853968    -1.879794    -1.990560      19.55
 O      -2.253996    -3.113028    -1.615337     289.42
 H      -2.869618    -3.707112    -1.954518      23.08
 C      -3.750076    -2.758646     0.012188      96.44
 H      -3.284806    -3.164846     1.013808      16.72
 O      -4.576669    -1.769856     0.817016     343.88
 H      -4.460183    -1.933654     1.690503      29.48
 C      -4.721533    -3.920461    -0.401169     107.89
 O      -4.351399    -5.081309    -1.081053     378.75
 H      -3.460977    -5.439706    -0.841823      29.61
 H      -5.672570    -3.546605    -0.816822      26.95
 H      -5.116727    -4.136743     0.519431      29.28
55
name = lig-etoh-frame_818
 C       2.569342     2.130415    -2.326940      59.13
 H       2.131653     2.790664    -3.030776      22.44
 C       3.609599     1.666175    -0.036785      54.04
 H       4.071931     1.851560     0.890448      20.38
 C       3.973529     0.438141    -0.551139      25.58
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 O       4.723609    -0.436610     0.163042     236.23
 C       5.270419    -0.039758     1.386306     119.58
 H       4.588014    -0.022140     2.253765      25.39
 H       5.735025     0.973707     1.025836      25.27
 H       6.124852    -0.675554     1.778385      25.84
 C       3.636631    -0.152257    -1.804255      25.13
 O       4.045399    -1.323154    -2.475601     210.45
 H       4.951655    -1.734081    -2.215148      24.53
 C       3.139013     0.827009    -2.683950      36.09
 H       2.813469     0.548257    -3.784086      22.04
 C       2.775257     2.486836    -0.819765      18.27
 C       2.133825     3.789480    -0.377500      95.56
 H       2.679471     4.588527    -1.115897      19.97
 O       2.331909     4.088011     1.001253     308.18
 H       3.194596     4.404857     0.992761      29.90
 C       0.417796     3.721377    -0.458313      31.68
 H      -0.177108     3.242175    -1.276447      19.26
 C      -0.415467     4.970222    -0.141174     109.21
 O       0.033593     6.076844    -0.999191     260.44
 H       0.177522     5.587969    -1.998477      23.62
 H      -0.057337     5.218918     0.857333      23.81
 H      -1.460801     4.720648    -0.157452      23.91
 C      -0.947951    -0.915108    -0.404750      46.22
 H      -0.665008    -1.858871    -0.076494      24.16
 C      -2.863311     0.434217    -0.973370      44.79
 H      -3.905141     0.328791    -1.367512      22.60
 C      -2.196500     1.685921    -0.559521      -6.80
 O      -2.816842     3.042425    -0.775468     199.69
 C      -4.157420     3.041699    -1.139026     147.84
 H      -4.994150     3.011080    -0.451501      27.32
 H      -4.563161     3.979714    -1.251697      27.20
 H      -4.404347     2.412413    -1.970037      27.98
 C      -0.851104     1.587033    -0.042611      21.41
 O      -0.097726     2.543982     0.574479     111.19
 C      -0.297610     0.347834    -0.015277      38.44
 H       0.834773     0.168644     0.029466      21.35
 C      -2.271196    -0.902359    -0.834507      -1.41
 C      -3.116667    -2.098584    -1.154235      85.99
 H      -3.824216    -1.694633    -1.875036      21.66
 O      -2.254750    -3.084105    -1.605371     261.94
 H      -2.965039    -3.740856    -1.958606      17.96
 C      -3.822561    -2.769492     0.134699      79.74
 H      -3.043421    -3.145319     0.838133      19.82
 O      -4.531745    -1.820671     0.797702     291.26
 H      -4.551360    -2.057351     1.900433      22.71
 C      -4.702014    -3.890574    -0.316946      72.49
 O      -4.368789    -5.080060    -1.092441     342.57
 H      -3.427924    -5.303703    -0.923206      27.85
 H      -5.408189    -3.391057    -1.048838      24.50
 H      -4.971103    -4.260049     0.822936      24.43
55
name = lig-etoh-frame_819
 C       2.582253     2.014205    -2.309197      81.65
 H       2.128056     2.644836    -3.130736      24.12
 C       3.556713     1.675547     0.017291      61.32
 H       4.153162     1.947824     0.923514      21.95
 C       3.977546     0.457972    -0.549646      28.14
 O       4.705030    -0.487999     0.200894     248.77
 C       5.341461    -0.041159     1.393861     124.52
 H       4.683139     0.276999     2.274417      24.33
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 H       5.832151     0.919443     1.335271      27.34
 H       6.098488    -0.768610     1.751997      26.13
 C       3.673849    -0.049681    -1.821632      20.76
 O       4.006510    -1.306737    -2.492860     214.75
 H       4.827514    -1.723118    -2.076686      24.71
 C       3.133872     0.849464    -2.729952      47.09
 H       2.905790     0.583925    -3.696158      23.15
 C       2.779307     2.485900    -0.834699      38.80
 C       2.076607     3.703654    -0.388130     113.87
 H       2.569253     4.384366    -1.125631      19.49
 O       2.360162     4.076076     1.034696     281.53
 H       3.266261     4.631032     1.202097      24.89
 C       0.471880     3.759451    -0.452002      26.32
 H       0.056086     3.243442    -1.367687      18.50
 C      -0.453945     5.033322    -0.119039     104.41
 O       0.055225     6.063497    -1.019939     280.81
 H       0.042468     5.752711    -1.923228      29.50
 H      -0.265335     5.292759     0.950541      23.70
 H      -1.491461     4.717058    -0.483413      20.78
 C      -0.955277    -0.931375    -0.385776     -33.04
 H      -0.232243    -1.930907    -0.296004      19.54
 C      -2.865336     0.453954    -0.977718      55.98
 H      -3.820953     0.833674    -1.373275      20.75
 C      -2.269381     1.579706    -0.587209       0.01
 O      -2.784761     3.048168    -0.742462     155.41
 C      -4.172815     3.028979    -1.164906      90.57
 H      -4.791576     2.536042    -0.188016      24.03
 H      -4.212540     4.218540    -1.467042      22.55
 H      -4.247958     2.297929    -2.168201      22.59
 C      -0.895877     1.618748    -0.009752       1.57
 O      -0.089696     2.540503     0.569200     103.25
 C      -0.222599     0.358080    -0.022533       5.68
 H       0.910608     0.290583     0.116898      21.57
 C      -2.373327    -0.903070    -0.910170      13.63
 C      -3.095403    -2.047897    -1.129277      94.14
 H      -3.959328    -1.712392    -1.806107      21.83
 O      -2.250856    -3.093539    -1.638453     217.22
 H      -2.741953    -3.974276    -1.999957      16.63
 C      -3.805618    -2.781635     0.228208      59.84
 H      -2.684934    -3.125732     0.399405      20.91
 O      -4.527600    -1.837230     0.826114     331.01
 H      -4.638260    -2.151228     1.734231      25.84
 C      -4.739674    -3.888431    -0.201613     100.92
 O      -4.362439    -5.068904    -1.111436     333.20
 H      -3.366121    -5.415204    -0.933374      26.14
 H      -5.374165    -3.345565    -0.871866      26.52
 H      -5.177331    -4.328740     0.613018      27.67
55
name = lig-etoh-frame_820
 C       2.593424     1.975000    -2.213927      82.75
 H       2.068862     2.564634    -2.959472      25.85
 C       3.517746     1.683288     0.032608      82.11
 H       3.848723     2.208712     0.972969      23.47
 C       4.001731     0.414646    -0.527060      19.24
 O       4.698098    -0.543874     0.248207     203.69
 C       5.412501    -0.015364     1.436655     107.77
 H       4.648590     0.279904     2.154096      24.47
 H       6.146224     0.920785     1.435056      25.42
 H       5.992472    -0.911320     1.674365      25.83
 C       3.732098     0.023807    -1.887099      14.37
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 O       3.972032    -1.268131    -2.485464     100.25
 H       4.615148    -1.723716    -1.678594      19.94
 C       3.099024     0.864746    -2.779110      43.06
 H       3.082128     0.449390    -3.931504      20.96
 C       2.760717     2.434005    -0.915314      65.90
 C       2.008057     3.668086    -0.354412     119.26
 H       2.212976     4.604335    -1.126774      17.57
 O       2.395441     4.069660     1.057408     296.91
 H       3.184658     4.626270     1.265209      29.25
 C       0.493757     3.740625    -0.436627      38.11
 H       0.439128     3.460582    -1.534667      16.34
 C      -0.435187     5.055865    -0.137300     105.46
 O       0.073935     6.063986    -1.004425     266.67
 H      -0.014104     5.859623    -2.041844      25.56
 H      -0.621392     5.448932     0.895891      23.20
 H      -1.405106     4.786761    -0.520793      21.55
 C      -0.949191    -0.911350    -0.364714      33.64
 H      -0.216748    -1.612412    -0.665857      21.22
 C      -2.922685     0.454704    -1.003406      62.10
 H      -3.841340     0.850356    -1.448511      19.69
 C      -2.242478     1.606216    -0.563891       5.20
 O      -2.739764     2.980589    -0.707210     179.32
 C      -4.180660     3.030490    -1.186199     126.23
 H      -4.510336     2.384613    -0.479992      26.51
 H      -4.199566     3.978267    -1.542726      26.42
 H      -4.272915     2.503743    -2.090069      27.10
 C      -0.934663     1.574113     0.009049       1.05
 O      -0.074952     2.597287     0.556618      60.02
 C      -0.207425     0.291979    -0.059733      -9.35
 H       0.832655     0.419211     0.285184      20.48
 C      -2.334084    -0.798111    -0.908125      25.37
 C      -3.181874    -2.079214    -1.125439      86.62
 H      -4.025277    -1.982163    -1.772427      21.83
 O      -2.224764    -3.121606    -1.703062     262.40
 H      -2.643239    -3.890041    -1.887496      23.78
 C      -3.671619    -2.809209     0.205155      81.03
 H      -2.730055    -3.106811     0.603592      24.08
 O      -4.546813    -1.818436     0.887741     281.85
 H      -4.702973    -2.168685     1.881234      24.83
 C      -4.777588    -3.923406    -0.136803      88.33
 O      -4.330672    -5.041457    -1.122235     312.50
 H      -3.586041    -5.542340    -0.836359      31.05
 H      -5.659708    -3.354210    -0.622536      25.93
 H      -5.590923    -4.442738     0.629017      26.32
55
name = lig-etoh-frame_821
 C       2.554280     2.014987    -2.178575      59.85
 H       1.902775     2.702332    -2.734377      20.75
 C       3.496517     1.665311    -0.005747      46.81
 H       3.472750     2.200237     0.943771      17.21
 C       4.022644     0.379313    -0.482404      26.32
 O       4.704568    -0.574060     0.288399     213.09
 C       5.484676     0.006578     1.482017      99.14
 H       4.615084     0.185205     2.176406      24.95
 H       6.220890     0.691955     1.176323      28.20
 H       5.869753    -1.014214     1.839624      25.74
 C       3.795575     0.043024    -1.956340      19.93
 O       3.963672    -1.224161    -2.414983     174.73
 H       4.346711    -1.717138    -1.793834      26.36
 C       3.088821     0.832633    -2.847340      61.87
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 H       3.101747     0.593000    -3.802644      26.58
 C       2.728862     2.388902    -0.925609      52.05
 C       1.972953     3.724715    -0.295543     112.96
 H       2.022851     4.669552    -0.932052      21.82
 O       2.410882     4.047426     1.067446     278.56
 H       3.234248     4.532081     1.063727      32.19
 C       0.475056     3.680151    -0.393784      66.52
 H       0.462068     3.675619    -1.529085      16.93
 C      -0.393790     5.035229    -0.199592     108.91
 O       0.100957     6.094158    -0.981538     264.81
 H       0.034983     5.842626    -1.999747      27.05
 H      -0.662091     5.487955     0.757909      23.61
 H      -1.437646     4.712756    -0.491792      22.13
 C      -0.941086    -0.840484    -0.388096      71.55
 H      -0.357408    -1.734722    -0.881540      20.21
 C      -2.980261     0.492228    -1.025007      42.00
 H      -3.961115     0.366580    -1.555592      18.14
 C      -2.174811     1.707628    -0.521853      12.36
 O      -2.698235     2.882853    -0.685835     159.31
 C      -4.110070     3.004001    -1.212653      77.44
 H      -4.913907     2.429372    -0.444245      22.58
 H      -4.550852     4.182184    -1.334469      22.44
 H      -4.317190     2.526889    -2.356803      21.97
 C      -0.912402     1.487778     0.024681      25.17
 O      -0.081341     2.667864     0.513480      97.21
 C      -0.268073     0.256065    -0.084123      29.98
 H       0.785261     0.350517     0.434859      19.48
 C      -2.269273    -0.726819    -0.871530     -13.47
 C      -3.236444    -2.163093    -1.126846      65.95
 H      -4.134083    -2.129131    -1.844497      19.26
 O      -2.187629    -3.115296    -1.772245     181.15
 H      -2.837376    -4.014726    -1.772035      14.30
 C      -3.598373    -2.821876     0.167836      81.92
 H      -2.892271    -3.141429     1.099277      17.74
 O      -4.554824    -1.797850     0.948057     258.75
 H      -4.534460    -2.167874     1.963800      23.78
 C      -4.839302    -3.992183    -0.103919      94.80
 O      -4.320433    -4.985748    -1.125741     295.87
 H      -3.712991    -5.650364    -0.600886      28.39
 H      -5.613285    -3.427080    -0.571108      30.30
 H      -5.301530    -4.402589     0.728802      30.66
55
name = lig-etoh-frame_822
 C       2.483006     2.056634    -2.272050      15.63
 H       1.763251     2.796306    -2.707197      17.04
 C       3.493998     1.601852    -0.058513      65.84
 H       3.301612     1.869454     1.051695      17.54
 C       4.023925     0.381793    -0.464770      28.58
 O       4.718239    -0.583751     0.320576     230.07
 C       5.497975    -0.051298     1.517229      99.01
 H       4.859916     0.447282     2.259976      27.49
 H       6.286261     0.617169     0.936385      25.69
 H       5.927458    -0.872265     2.045357      28.08
 C       3.844673     0.049735    -1.952763      22.13
 O       3.962935    -1.201276    -2.360479     137.41
 H       4.446783    -1.918029    -1.695011      20.28
 C       3.078888     0.870106    -2.834730      59.10
 H       2.942372     0.690426    -4.046752      22.72
 C       2.681929     2.410062    -0.846538      54.68
 C       1.967755     3.785241    -0.227090     101.28
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 H       2.235112     4.782053    -0.868443      20.26
 O       2.417824     4.019376     1.074730     264.80
 H       3.398549     4.375732     0.818968      28.24
 C       0.431337     3.645347    -0.350620      88.48
 H       0.135527     3.438468    -1.413515      18.00
 C      -0.374683     4.983540    -0.258807     106.19
 O       0.133493     6.132305    -0.969572     275.82
 H       0.198574     5.859833    -1.914297      30.40
 H      -0.362250     5.366823     0.818928      23.43
 H      -1.379710     4.649097    -0.572106      22.54
 C      -0.951031    -0.852677    -0.487855      65.28
 H      -0.636436    -1.919202    -0.656599      21.16
 C      -2.964743     0.526201    -1.013599      64.48
 H      -3.884940     0.164776    -1.455267      18.55
 C      -2.166221     1.688239    -0.522444       7.85
 O      -2.711149     2.868886    -0.681525     176.10
 C      -4.084613     2.980305    -1.241652     128.91
 H      -4.929856     2.687371    -0.735076      27.60
 H      -4.418459     3.900756    -0.913896      26.56
 H      -4.122277     2.655491    -2.174717      28.33
 C      -0.857946     1.483369     0.034740      31.27
 O      -0.119607     2.700047     0.462001     194.93
 C      -0.272494     0.282922    -0.037485      62.20
 H       0.682653     0.116050     0.293461      20.94
 C      -2.294013    -0.705507    -0.844670     -28.45
 C      -3.174493    -2.227566    -1.138221      65.67
 H      -4.049845    -2.058644    -1.739270      21.24
 O      -2.199186    -3.117586    -1.835255     249.75
 H      -2.676723    -3.977013    -1.704692      19.12
 C      -3.657058    -2.839715     0.217732      90.11
 H      -3.037380    -3.122470     0.986988      20.08
 O      -4.538026    -1.785916     0.978238     306.12
 H      -4.386419    -2.121741     1.955346      23.35
 C      -4.825922    -4.032519    -0.107236      71.37
 O      -4.323235    -4.929874    -1.106655     298.60
 H      -3.861556    -5.648242    -0.560791      28.83
 H      -5.601271    -3.433915    -0.668202      27.12
 H      -4.883787    -4.508380     1.030336      25.82
55
name = lig-etoh-frame_823
 C       2.418247     2.115379    -2.320621      48.40
 H       1.779052     2.692418    -2.977983      20.00
 C       3.463456     1.544319    -0.047498      67.03
 H       3.466736     1.478679     1.008485      18.54
 C       4.033611     0.373783    -0.514464      21.40
 O       4.719931    -0.586019     0.361490     266.41
 C       5.499224    -0.092489     1.507162     123.12
 H       5.155048     0.794651     2.163326      26.38
 H       6.250879     0.493388     1.100362      29.23
 H       6.073534    -0.869211     2.146315      26.66
 C       3.857832     0.080863    -1.875086      19.96
 O       3.978379    -1.246791    -2.324031     129.89
 H       4.706363    -1.698915    -1.705960      20.60
 C       3.057543     0.966237    -2.816112      28.77
 H       2.818277     0.682244    -3.773438      21.34
 C       2.617020     2.461157    -0.828755      82.61
 C       1.976590     3.801747    -0.215293     113.22
 H       2.399820     4.650245    -0.873407      21.95
 O       2.446586     4.004392     1.088472     300.49
 H       3.398370     4.128389     1.033279      31.87
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 C       0.394283     3.656130    -0.394400      74.27
 H       0.080470     3.041701    -1.295387      18.33
 C      -0.355814     4.945694    -0.265083     111.55
 O       0.162766     6.152131    -0.954779     237.50
 H       0.431974     5.931181    -2.005411      24.49
 H      -0.171680     5.114069     0.785214      24.43
 H      -1.377691     4.766841    -0.612831      22.92
 C      -0.997108    -0.897308    -0.586311      21.29
 H      -0.616821    -1.949008    -0.333992      21.56
 C      -2.884894     0.514512    -0.966189      72.60
 H      -3.966464     0.606857    -1.308309      22.13
 C      -2.201325     1.571731    -0.553327       9.46
 O      -2.758087     2.916941    -0.673045     168.38
 C      -4.052097     2.983739    -1.216967      88.43
 H      -4.920079     2.235265    -0.731391      23.11
 H      -4.079870     4.163608    -0.911752      21.71
 H      -3.934861     2.806752    -2.510334      22.35
 C      -0.827778     1.585576     0.016943      11.27
 O      -0.190403     2.672994     0.471230     192.47
 C      -0.235999     0.255634     0.020217      12.31
 H       0.926277    -0.047918     0.185629      18.20
 C      -2.362513    -0.763545    -0.841700       6.67
 C      -3.043769    -2.226154    -1.117144      76.26
 H      -3.973641    -1.906962    -1.715940      21.82
 O      -2.233939    -3.117262    -1.880722     260.61
 H      -2.487050    -4.059865    -1.767470      19.62
 C      -3.817298    -2.836165     0.261599      68.41
 H      -2.773644    -3.265007     0.855243      19.97
 O      -4.499107    -1.790688     0.966031     316.57
 H      -4.359710    -1.977510     2.045837      22.88
 C      -4.747175    -4.014654    -0.081917     111.24
 O      -4.329238    -4.900747    -1.080600     360.04
 H      -3.865441    -5.638331    -0.764212      33.86
 H      -5.722269    -3.597657    -0.381815      27.36
 H      -4.782042    -4.516652     0.807746      28.11
55
name = lig-etoh-frame_824
 C       2.384133     2.181918    -2.286396      72.45
 H       1.858403     2.619209    -3.192868      21.95
 C       3.385534     1.528990    -0.031414      46.16
 H       3.616694     1.470823     1.107660      17.73
 C       4.068889     0.361349    -0.561591      10.62
 O       4.700397    -0.584279     0.398075     236.05
 C       5.526145    -0.083972     1.493362     119.38
 H       5.115578     0.764039     2.008120      26.31
 H       6.568190     0.412794     1.075890      25.44
 H       5.855500    -0.926050     2.038437      26.84
 C       3.812399     0.093243    -1.853709      21.17
 O       4.018614    -1.284619    -2.289280     133.34
 H       4.861084    -1.567790    -1.826957      23.64
 C       3.057585     1.046546    -2.720252      39.48
 H       2.767292     0.512594    -3.752631      21.07
 C       2.569731     2.484063    -0.858416      38.77
 C       1.997689     3.749972    -0.247974     103.78
 H       2.421587     4.569162    -1.024870      19.90
 O       2.462313     3.993294     1.126458     307.51
 H       3.439107     3.981865     1.311694      26.83
 C       0.384834     3.640413    -0.506036      49.60
 H       0.404079     3.121656    -1.448507      20.40
 C      -0.333854     4.939929    -0.272435     101.52
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 O       0.204914     6.141854    -0.945100     266.10
 H       0.371472     5.962363    -1.827782      31.66
 H      -0.250304     5.073262     0.858844      22.35
 H      -1.455357     4.955460    -0.477210      22.22
 C      -1.012939    -0.907292    -0.606081      21.73
 H      -0.498231    -1.806064    -0.100983      21.75
 C      -2.887947     0.446483    -0.937618      65.75
 H      -3.785673     1.015807    -1.112536      22.36
 C      -2.177120     1.568959    -0.553212       4.03
 O      -2.774193     2.919190    -0.643660     209.50
 C      -4.038240     3.032417    -1.220087     144.18
 H      -4.514455     2.198772    -0.918225      27.08
 H      -4.237785     4.067964    -1.248092      25.76
 H      -4.016092     3.018474    -2.213322      29.89
 C      -0.824630     1.591607    -0.042119      -4.79
 O      -0.259063     2.656543     0.554778     142.15
 C      -0.202153     0.198746     0.026784       5.52
 H       0.792175     0.114755     0.182711      21.01
 C      -2.389588    -0.915451    -0.855720      24.34
 C      -3.003682    -2.160474    -1.085465      94.63
 H      -3.800243    -1.891085    -1.751215      22.55
 O      -2.257796    -3.107314    -1.918845     213.04
 H      -2.433146    -4.180881    -1.740744      15.51
 C      -3.875126    -2.825744     0.286223      96.22
 H      -3.017451    -3.239309     0.594251      25.47
 O      -4.452540    -1.798532     0.953761     369.21
 H      -4.429116    -1.926793     1.881613      28.71
 C      -4.689520    -3.973633    -0.038513      98.79
 O      -4.330955    -4.884822    -1.090617     300.89
 H      -3.692384    -5.683518    -0.885349      28.65
 H      -5.801634    -3.767172    -0.061037      25.77
 H      -4.919904    -4.704146     0.960865      24.52
55
name = lig-etoh-frame_825
 C       2.391280     2.222640    -2.229529      72.77
 H       1.901998     2.782129    -2.999254      23.59
 C       3.311749     1.525341    -0.029308      54.96
 H       3.455303     1.904515     0.954468      20.10
 C       4.090447     0.397104    -0.516332       0.53
 O       4.669495    -0.566758     0.399668     233.59
 C       5.595847    -0.039941     1.432871     111.88
 H       4.949779     0.660949     2.052116      22.80
 H       6.546061     0.125748     1.087016      26.91
 H       5.527000    -1.041594     2.066884      24.08
 C       3.741233     0.055074    -1.904191      11.35
 O       4.049507    -1.279993    -2.265644      84.83
 H       5.087503    -1.612545    -1.941054      21.86
 C       3.070012     1.034859    -2.627416      55.01
 H       2.839272     0.569243    -3.594477      23.02
 C       2.569194     2.455109    -0.871763      15.94
 C       2.033006     3.685010    -0.279237      78.91
 H       2.295814     4.568008    -1.004596      19.19
 O       2.439011     3.985119     1.154004     310.37
 H       3.489589     3.901922     1.376125      25.20
 C       0.419327     3.616245    -0.574382      24.13
 H       0.487994     3.357732    -1.697799      14.85
 C      -0.336704     4.973003    -0.267365     102.57
 O       0.248091     6.108968    -0.904262     233.24
 H       0.265651     5.875393    -1.992441      24.92
 H      -0.301512     5.177507     0.783255      23.05
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 H      -1.396047     4.926515    -0.396245      23.07
 C      -0.950511    -0.898334    -0.512380      46.24
 H      -0.489718    -1.847319    -0.288592      23.99
 C      -2.909194     0.376586    -0.907279      30.12
 H      -3.974792     0.670365    -1.160393      21.57
 C      -2.115537     1.633057    -0.539024       2.86
 O      -2.735969     2.892515    -0.595156     177.97
 C      -4.014437     3.102741    -1.246304      94.65
 H      -4.810509     2.255220    -0.864325      23.31
 H      -4.728212     4.118063    -1.110294      22.66
 H      -4.004992     2.936923    -2.540424      22.70
 C      -0.825301     1.472698    -0.098572       9.15
 O      -0.299652     2.675497     0.625902      62.83
 C      -0.266047     0.202162    -0.041737      51.40
 H       0.877242     0.219200     0.321634      19.42
 C      -2.336926    -0.972352    -0.854336      10.16
 C      -3.104378    -2.158235    -1.094722      92.25
 H      -3.910199    -1.914524    -1.846403      19.92
 O      -2.257079    -3.109864    -1.944062     266.06
 H      -2.563776    -3.911735    -1.634842      20.57
 C      -3.825071    -2.799825     0.235653      72.81
 H      -2.829371    -3.287031     0.910664      18.47
 O      -4.424379    -1.775630     0.935484     283.53
 H      -4.512385    -2.046490     2.051783      22.19
 C      -4.730729    -4.029935     0.055567     100.58
 O      -4.327749    -4.877303    -1.124526     361.75
 H      -3.561254    -5.451615    -0.816054      28.72
 H      -5.799131    -3.746194    -0.130478      26.39
 H      -4.734973    -4.587808     0.923296      28.64
55
name = lig-etoh-frame_826
 C       2.449233     2.206468    -2.180085      47.83
 H       1.923661     3.029843    -2.742085      22.22
 C       3.272638     1.538318    -0.039206      68.33
 H       3.276852     2.203966     0.886927      18.54
 C       4.047660     0.450201    -0.452503      17.20
 O       4.644075    -0.518812     0.353812     233.53
 C       5.587111    -0.061997     1.402768     114.70
 H       5.145496     0.745527     2.038620      23.80
 H       6.698092     0.083861     1.043864      24.83
 H       5.484408    -0.863708     2.080558      26.83
 C       3.721669    -0.002891    -1.861729      16.46
 O       4.084378    -1.256478    -2.272815     208.81
 H       4.830656    -1.570210    -1.906432      27.00
 C       3.058167     0.977339    -2.599067      50.58
 H       2.851356     0.717835    -3.700591      21.51
 C       2.607634     2.402875    -0.854992      32.11
 C       2.041659     3.649666    -0.272138     102.91
 H       2.233860     4.669001    -0.848259      18.27
 O       2.392644     3.968437     1.153894     350.97
 H       3.314340     4.022693     1.174887      31.07
 C       0.471359     3.634601    -0.557904      36.52
 H       0.169600     3.416822    -1.576682      17.49
 C      -0.330440     4.991928    -0.246288      97.41
 O       0.293642     6.058724    -0.903566     248.31
 H       0.189121     5.942237    -1.862333      30.59
 H      -0.187345     5.251480     0.849661      23.15
 H      -1.428512     4.751450    -0.558490      21.65
 C      -0.891681    -0.954255    -0.386142      53.58
 H      -0.383805    -1.997375    -0.680103      18.59
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 C      -2.915834     0.345277    -0.872503      44.36
 H      -3.931120     0.037820    -1.203131      18.61
 C      -2.149734     1.623605    -0.568345       4.52
 O      -2.698686     2.887324    -0.545357     144.65
 C      -4.057893     3.132222    -1.317443     121.59
 H      -4.863125     2.585743    -0.945471      26.45
 H      -4.536166     3.908492    -0.778969      25.09
 H      -3.909396     2.938745    -2.230872      28.07
 C      -0.832010     1.424404    -0.098760      16.56
 O      -0.313748     2.675627     0.618129      58.72
 C      -0.276183     0.228695    -0.109382      61.31
 H       0.638813     0.165462     0.374068      20.98
 C      -2.249811    -0.883130    -0.831339     -10.42
 C      -3.254143    -2.214941    -1.152244      67.63
 H      -4.113842    -1.915263    -1.767959      21.25
 O      -2.263341    -3.094515    -1.939740     223.05
 H      -2.738428    -3.958440    -1.631921      16.86
 C      -3.676981    -2.813931     0.197051      99.96
 H      -3.019002    -3.041820     0.892977      22.57
 O      -4.417755    -1.737668     0.954701     357.04
 H      -4.507343    -2.112095     1.764069      29.11
 C      -4.785523    -4.088664     0.093750      72.26
 O      -4.320202    -4.867721    -1.136524     339.04
 H      -3.525854    -5.290991    -0.815477      28.29
 H      -5.728320    -3.661412    -0.267558      27.01
 H      -4.570684    -4.650946     1.125296      25.87
55
name = lig-etoh-frame_827
 C       2.530519     2.151775    -2.167117      41.47
 H       2.079788     2.988614    -2.693850      19.34
 C       3.282378     1.576283     0.018826      43.24
 H       3.347759     1.907109     1.059579      18.88
 C       3.953376     0.465003    -0.435295      37.66
 O       4.640424    -0.456792     0.305642     268.15
 C       5.558518    -0.088140     1.384705     127.22
 H       5.424430     0.952297     1.825164      25.40
 H       6.554820     0.125896     1.039614      27.82
 H       5.663479    -0.916967     2.189871      25.50
 C       3.728619    -0.015989    -1.733131      26.62
 O       4.086300    -1.219027    -2.316599     148.23
 H       4.846335    -1.685398    -1.556869      19.34
 C       3.011665     0.909983    -2.655957      64.92
 H       2.940002     0.857681    -3.812640      23.88
 C       2.636470     2.396702    -0.828465      35.44
 C       1.998258     3.663948    -0.241215     110.05
 H       2.366058     4.623210    -0.820200      18.47
 O       2.318344     3.939119     1.124118     290.61
 H       3.313555     4.303837     1.070811      27.29
 C       0.483414     3.676286    -0.448490      43.21
 H      -0.029987     3.225791    -1.350204      17.63
 C      -0.308841     4.964140    -0.202566     113.59
 O       0.336721     6.030274    -0.915027     253.31
 H       0.226816     5.954466    -1.928780      27.51
 H      -0.229260     5.203958     0.842989      24.66
 H      -1.247668     4.760554    -0.593161      24.25
 C      -0.877888    -1.084162    -0.330815      52.33
 H      -0.287731    -1.823255    -0.698539      21.57
 C      -2.901533     0.347335    -0.844599      66.25
 H      -3.884847    -0.017216    -1.192847      18.46
 C      -2.255128     1.547882    -0.613133       6.15
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 O      -2.701343     2.889419    -0.514453     123.45
 C      -4.078848     3.139785    -1.276720      74.34
 H      -4.879181     2.304490    -1.009203      22.19
 H      -4.092069     4.254679    -0.775955      21.49
 H      -3.797688     3.111452    -2.575110      21.46
 C      -0.892240     1.516512    -0.064939      -4.58
 O      -0.303838     2.644473     0.541624     127.07
 C      -0.210994     0.210568    -0.131188       2.22
 H       0.800153     0.125292     0.409920      18.46
 C      -2.191186    -0.821201    -0.800739     -15.33
 C      -3.295917    -2.227989    -1.200802      48.13
 H      -4.269429    -1.947889    -1.691527      20.84
 O      -2.313165    -3.082782    -1.899449     183.71
 H      -2.734866    -4.081669    -2.042624      17.01
 C      -3.629483    -2.825359     0.172567      63.87
 H      -2.624131    -3.035931     0.915356      17.61
 O      -4.410299    -1.700651     0.932685     269.78
 H      -4.570280    -2.208778     1.913077      23.60
 C      -4.753116    -4.107753     0.080618      77.54
 O      -4.321511    -4.862832    -1.116979     337.19
 H      -3.429271    -5.416959    -0.903631      25.27
 H      -5.754207    -3.617824    -0.150454      27.44
 H      -4.781779    -4.675969     1.056617      26.98
55
name = lig-etoh-frame_828
 C       2.613618     2.080216    -2.183242      52.38
 H       2.223323     2.789112    -2.940113      19.37
 C       3.327161     1.609169     0.143468      50.67
 H       3.465110     1.550280     1.242869      18.38
 C       3.859916     0.438295    -0.430265      28.12
 O       4.662847    -0.421722     0.294764     270.35
 C       5.534832    -0.084387     1.376849     126.89
 H       5.432444     0.988073     1.647544      27.18
 H       6.591594     0.013298     0.831738      25.84
 H       5.687122    -0.844626     2.133818      27.62
 C       3.685411     0.020607    -1.704697      21.90
 O       4.115653    -1.189361    -2.318990     221.28
 H       4.540413    -1.726111    -1.670744      25.59
 C       2.983769     0.856575    -2.707828      52.64
 H       3.038486     0.689408    -3.758884      24.36
 C       2.637148     2.447718    -0.778363      56.84
 C       1.942669     3.698507    -0.227497     128.95
 H       2.479568     4.445101    -0.949733      22.01
 O       2.263744     3.912103     1.096336     301.34
 H       3.057929     4.546680     1.224042      30.05
 C       0.428887     3.670932    -0.329617      72.11
 H       0.271712     3.173532    -1.286782      19.53
 C      -0.254151     4.934914    -0.164692     109.61
 O       0.379157     6.024937    -0.925127     230.46
 H       0.319508     5.780768    -1.988828      24.84
 H      -0.387809     5.216525     0.924294      24.63
 H      -1.361571     4.842732    -0.540152      22.12
 C      -0.878410    -1.112921    -0.324256      37.14
 H      -0.102443    -2.009063    -0.583366      19.17
 C      -2.911871     0.343734    -0.842290      69.02
 H      -3.957587     0.490882    -1.154131      21.15
 C      -2.306690     1.537646    -0.602473       8.19
 O      -2.756440     2.861838    -0.521517     199.64
 C      -4.035764     3.165346    -1.225376     139.06
 H      -4.685178     2.375527    -1.090110      25.65
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 H      -4.019029     4.217249    -1.178885      25.10
 H      -3.953875     3.329011    -2.165396      29.38
 C      -0.942813     1.551316    -0.044402     -10.82
 O      -0.278659     2.608950     0.462261     153.30
 C      -0.149712     0.196128    -0.090987     -24.91
 H       0.939709     0.229254     0.193199      19.18
 C      -2.184336    -0.887155    -0.781872      14.82
 C      -3.238088    -2.206487    -1.201145      71.67
 H      -4.191946    -1.984799    -1.728849      22.23
 O      -2.381253    -3.090013    -1.876672     296.06
 H      -2.713535    -3.796417    -2.281861      28.34
 C      -3.637724    -2.831378     0.218616      85.30
 H      -2.682481    -3.072011     0.459406      26.11
 O      -4.388984    -1.708449     0.909775     314.92
 H      -4.614264    -1.979867     1.863338      26.36
 C      -4.659190    -4.071530     0.034695     104.14
 O      -4.321401    -4.883494    -1.084139     369.25
 H      -3.611706    -5.494437    -0.960172      31.73
 H      -5.656637    -3.671724    -0.046185      27.62
 H      -4.942077    -4.744544     0.971119      26.12
55
name = lig-etoh-frame_829
 C       2.663665     2.052792    -2.200764      71.39
 H       2.308873     2.646855    -3.072999      21.43
 C       3.363147     1.622698     0.234816      62.39
 H       3.435198     1.558764     1.359436      17.83
 C       3.799684     0.409931    -0.383293      13.62
 O       4.679576    -0.436471     0.299543     243.36
 C       5.565089    -0.026359     1.318705     122.85
 H       5.296590     0.941919     1.756628      28.26
 H       6.516832    -0.121741     0.854827      27.04
 H       5.493819    -0.805929     2.160977      28.20
 C       3.606397     0.033592    -1.806453      18.63
 O       4.128916    -1.146595    -2.310485     182.52
 H       4.548468    -1.822340    -1.661777      22.23
 C       2.998904     0.805065    -2.685622      54.65
 H       3.088153     0.346138    -3.810528      20.90
 C       2.643347     2.474711    -0.713188      83.39
 C       1.922750     3.715065    -0.241742     124.85
 H       2.271554     4.517254    -1.002241      22.78
 O       2.223086     3.910077     1.115278     315.60
 H       2.819269     4.550962     1.336430      35.25
 C       0.375083     3.589478    -0.293578      79.36
 H       0.500131     3.417612    -1.441890      18.35
 C      -0.263563     4.965821    -0.134595     117.70
 O       0.418485     6.006922    -0.935010     260.37
 H       0.412163     5.680333    -1.822496      32.35
 H      -0.354510     5.298408     0.899546      25.55
 H      -1.269210     4.900555    -0.417390      25.40
 C      -0.823945    -1.051910    -0.352778      41.97
 H      -0.406617    -1.993238    -0.288168      23.24
 C      -2.937335     0.329717    -0.860067      31.03
 H      -3.938240     0.722703    -1.123788      20.10
 C      -2.256353     1.588513    -0.525008      10.44
 O      -2.837285     2.824443    -0.550770     201.55
 C      -3.946565     3.206134    -1.165690     108.20
 H      -4.918352     2.541655    -0.922324      23.06
 H      -4.406147     4.343122    -0.987063      22.51
 H      -3.856341     3.185612    -2.514347      21.78
 C      -0.940206     1.451117    -0.061076       3.05
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 O      -0.242485     2.592412     0.429567     192.68
 C      -0.166232     0.210259    -0.038764      46.08
 H       0.918582     0.322665    -0.008893      21.77
 C      -2.270131    -1.016757    -0.790037     -15.80
 C      -3.156929    -2.155661    -1.145424      98.85
 H      -3.966144    -1.846609    -1.828144      20.95
 O      -2.405288    -3.093854    -1.870903     228.00
 H      -3.053533    -3.708101    -2.500267      21.50
 C      -3.711653    -2.818047     0.237978      71.91
 H      -2.564869    -3.229891     0.524219      21.77
 O      -4.350835    -1.737985     0.878787     318.84
 H      -4.553124    -1.903470     1.824348      27.75
 C      -4.553684    -4.022451     0.019753     102.49
 O      -4.337817    -4.915036    -1.073166     343.16
 H      -3.634679    -5.600196    -0.841936      28.52
 H      -5.609168    -3.576253    -0.254547      25.24
 H      -4.801302    -4.716274     0.895533      25.47
55
name = lig-etoh-frame_830
 C       2.670584     2.086279    -2.184876      45.23
 H       2.269885     2.781563    -2.910316      19.24
 C       3.362366     1.604754     0.254944      49.17
 H       3.345024     1.908494     1.291088      15.77
 C       3.771555     0.387078    -0.348978      11.64
 O       4.670095    -0.484583     0.285339     256.80
 C       5.589679     0.023545     1.288086     107.14
 H       5.281746     0.977674     1.850213      26.30
 H       6.697352     0.005309     0.989480      26.40
 H       5.318815    -0.684381     2.105655      27.72
 C       3.586501    -0.034954    -1.797501      11.28
 O       4.133918    -1.121326    -2.311444     155.43
 H       4.732838    -1.706101    -1.547662      18.78
 C       3.010402     0.781465    -2.705768      62.72
 H       2.947900     0.386858    -3.616423      24.98
 C       2.678947     2.452586    -0.700583      96.26
 C       1.930945     3.711406    -0.246843     120.05
 H       1.886013     4.725589    -0.847218      17.33
 O       2.177652     3.913497     1.168014     272.87
 H       2.877601     4.670658     1.385913      30.21
 C       0.367468     3.534206    -0.379038      64.65
 H       0.175775     3.565512    -1.453709      18.26
 C      -0.285834     5.020997    -0.103989      96.07
 O       0.448494     5.978016    -0.913513     169.01
 H       0.487652     5.625268    -1.983415      24.20
 H      -0.121443     5.406386     0.934437      23.90
 H      -1.395426     4.925062    -0.450530      23.36
 C      -0.841168    -0.949340    -0.398687      24.14
 H      -0.532701    -2.030369    -0.043244      20.64
 C      -2.919064     0.338923    -0.869398      28.44
 H      -3.975100     0.390096    -1.190932      23.29
 C      -2.209118     1.560378    -0.450905      18.73
 O      -2.863579     2.803499    -0.539673     214.44
 C      -3.978655     3.262319    -1.217655     145.53
 H      -4.878750     2.815894    -0.837621      26.71
 H      -4.362970     4.075666    -0.648249      24.99
 H      -3.793599     2.995725    -2.102494      28.59
 C      -0.881914     1.356928    -0.083164      20.65
 O      -0.214766     2.556592     0.435966     139.93
 C      -0.238319     0.211921    -0.007159      70.73
 H       0.918663     0.353553    -0.075239      19.22
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 C      -2.332747    -1.022920    -0.780540     -23.68
 C      -3.113072    -2.128738    -1.079645      89.27
 H      -3.833891    -1.602572    -1.771431      19.76
 O      -2.402913    -3.135017    -1.903359     246.68
 H      -3.282590    -3.441825    -2.333901      21.41
 C      -3.689629    -2.802478     0.217742     100.58
 H      -2.947284    -3.120178     0.892933      22.48
 O      -4.321828    -1.770027     0.851459     294.99
 H      -4.442079    -1.985830     1.947312      24.69
 C      -4.545712    -3.987258    -0.003339      94.63
 O      -4.339413    -4.962522    -1.080153     339.50
 H      -3.581223    -5.596362    -0.756727      26.29
 H      -5.415336    -3.531768    -0.361097      27.02
 H      -4.565118    -4.524675     1.008679      26.33
55
name = lig-etoh-frame_831
 C       2.650791     2.129536    -2.132695      32.55
 H       2.165339     3.005516    -2.662757      20.72
 C       3.318851     1.581380     0.201899      23.12
 H       3.382423     2.215712     1.165297      17.89
 C       3.776763     0.353075    -0.343416      14.78
 O       4.664431    -0.537621     0.266992     250.33
 C       5.588623     0.060393     1.301806     116.35
 H       5.343092     1.048769     1.599456      26.63
 H       6.688244     0.197114     1.129747      27.05
 H       5.488902    -0.664665     2.120146      26.72
 C       3.590489    -0.085171    -1.678689      31.04
 O       4.167697    -1.155248    -2.300990     237.57
 H       4.787735    -1.436181    -1.707942      28.45
 C       2.995188     0.845384    -2.685927      66.00
 H       2.708457     0.533310    -3.865681      21.81
 C       2.729633     2.424861    -0.762243      78.07
 C       1.917664     3.699111    -0.233293     113.13
 H       2.025737     4.701328    -0.694298      18.06
 O       2.132978     3.933189     1.232920     286.27
 H       2.946799     4.554660     1.245779      28.85
 C       0.360306     3.553498    -0.485163      46.73
 H      -0.190322     3.316461    -1.483825      18.03
 C      -0.301235     5.047970    -0.084580     102.06
 O       0.472519     5.944159    -0.918383     223.17
 H       0.420139     5.804199    -1.824415      31.35
 H      -0.001055     5.370452     0.916067      24.02
 H      -1.335836     5.031873    -0.325040      25.11
 C      -0.965125    -0.947671    -0.435933      71.13
 H      -0.430847    -1.804474    -0.067038      24.35
 C      -2.884671     0.334081    -0.869898      67.15
 H      -3.894661     0.114599    -1.215080      22.44
 C      -2.249682     1.473028    -0.432398      13.10
 O      -2.809920     2.783133    -0.469275     141.38
 C      -4.072008     3.275741    -1.207056      77.99
 H      -4.960525     2.577600    -0.918846      23.40
 H      -4.009095     4.371448    -0.697472      22.06
 H      -3.874746     3.049725    -2.524508      21.48
 C      -0.843104     1.419609    -0.085371       0.22
 O      -0.195886     2.496392     0.456864     152.74
 C      -0.237228     0.167862    -0.004968      47.40
 H       0.775210     0.199926     0.154982      22.25
 C      -2.261506    -0.850946    -0.731932      23.07
 C      -3.092122    -2.151990    -1.043636      77.12
 H      -3.964511    -1.702058    -1.541696      22.29
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 O      -2.416066    -3.165429    -1.938528     280.85
 H      -3.170735    -3.555649    -2.259523      25.00
 C      -3.593057    -2.788151     0.180170      91.18
 H      -2.917805    -3.040231     1.136938      18.49
 O      -4.343492    -1.775434     0.872935     353.57
 H      -4.350766    -2.028271     1.721708      29.50
 C      -4.590045    -3.993169    -0.046101      74.86
 O      -4.321931    -5.017913    -1.071857     360.65
 H      -3.529358    -5.499579    -0.896901      30.26
 H      -5.637863    -3.499681    -0.280622      26.27
 H      -4.544517    -4.282710     1.087010      25.38
55
name = lig-etoh-frame_832
 C       2.605226     2.168776    -2.110200      56.23
 H       2.134922     2.965853    -2.632005      22.55
 C       3.268741     1.578179     0.119650      58.81
 H       3.529791     2.015936     1.033668      21.52
 C       3.812303     0.312934    -0.334380      15.15
 O       4.691650    -0.583129     0.280025     242.94
 C       5.570228     0.081422     1.327583     107.08
 H       5.193193     1.172003     1.379587      25.80
 H       6.629848     0.185669     0.927737      26.56
 H       5.731983    -0.581102     2.259764      25.77
 C       3.554363    -0.055831    -1.648339      17.55
 O       4.186591    -1.197536    -2.286328     162.39
 H       5.153010    -1.512849    -1.725791      19.31
 C       2.962770     0.926477    -2.626326      43.38
 H       2.724340     0.797872    -3.570346      24.54
 C       2.754555     2.433682    -0.802305      46.36
 C       1.893531     3.665186    -0.222294     103.89
 H       2.554902     4.565334    -0.706792      18.57
 O       2.089928     3.951565     1.269925     297.80
 H       2.950638     4.303090     1.241531      30.02
 C       0.306196     3.602428    -0.542486      44.96
 H      -0.081722     3.078276    -1.415506      20.16
 C      -0.260261     5.023143    -0.099286     101.52
 O       0.491930     5.942158    -0.904609     202.11
 H       0.243645     5.829518    -1.973698      24.60
 H      -0.046137     5.214634     0.964650      23.76
 H      -1.373018     5.097901    -0.254398      23.85
 C      -0.981006    -0.976350    -0.407573      77.10
 H      -0.430014    -1.929681    -0.335680      23.33
 C      -2.904392     0.347332    -0.878169      78.95
 H      -3.938532     0.282966    -1.216325      24.41
 C      -2.294636     1.455409    -0.443238       1.64
 O      -2.755228     2.765076    -0.398217     119.57
 C      -4.120973     3.246713    -1.204802     111.91
 H      -4.935717     2.588758    -1.020057      25.55
 H      -3.883124     4.280951    -1.219929      24.22
 H      -4.094553     3.399423    -2.163022      28.78
 C      -0.844593     1.485054    -0.072849     -20.50
 O      -0.162733     2.467427     0.485929     151.23
 C      -0.230016     0.150522    -0.033124       1.34
 H       0.816876    -0.080755     0.544962      19.57
 C      -2.221616    -0.778096    -0.727122      40.56
 C      -3.044995    -2.147817    -1.044894      77.72
 H      -4.133401    -2.007151    -1.385073      20.83
 O      -2.426749    -3.158142    -1.959256     206.79
 H      -3.097062    -3.997860    -2.282957      17.21
 C      -3.502811    -2.800067     0.206753      88.60
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 H      -2.633093    -3.116343     0.742704      22.53
 O      -4.391325    -1.758822     0.879095     303.86
 H      -4.383529    -2.082286     1.921889      24.07
 C      -4.639021    -3.988791    -0.073726      91.32
 O      -4.318075    -5.060308    -1.049519     323.51
 H      -3.334196    -5.437474    -0.977356      25.60
 H      -5.612368    -3.653387    -0.179828      28.54
 H      -4.787191    -4.430862     0.965769      26.98
55
name = lig-etoh-frame_833
 C       2.542617     2.207885    -2.136178      42.30
 H       2.077172     2.880366    -2.917460      22.15
 C       3.278034     1.525161     0.058714      70.63
 H       3.578227     1.719883     1.152225      20.45
 C       3.847532     0.289265    -0.336793      12.50
 O       4.734637    -0.614502     0.330029     226.64
 C       5.565680     0.111432     1.328483     122.49
 H       5.137857     1.042323     1.486022      30.79
 H       6.450069     0.135413     0.641271      25.36
 H       5.690346    -0.342103     2.270304      29.08
 C       3.536683    -0.021928    -1.724368      19.47
 O       4.196862    -1.213911    -2.254416     199.67
 H       4.933664    -1.625066    -1.861465      25.31
 C       2.947764     0.979773    -2.501540      50.54
 H       2.795741     0.760410    -3.702887      21.09
 C       2.705114     2.496713    -0.756726      31.61
 C       1.925895     3.643382    -0.221244     107.39
 H       2.530095     4.352876    -0.735634      20.89
 O       2.034924     3.956633     1.263942     294.38
 H       3.127436     4.027317     1.432527      24.65
 C       0.279170     3.634028    -0.516896      48.94
 H       0.188047     3.188025    -1.551094      19.74
 C      -0.219759     4.962115    -0.142898     111.41
 O       0.500002     5.964412    -0.905156     237.51
 H       0.216658     5.765714    -1.837124      28.72
 H      -0.048880     5.030400     0.948047      24.31
 H      -1.316539     5.089701    -0.293946      24.69
 C      -0.854252    -1.011781    -0.332730      22.79
 H      -0.614825    -2.097717    -0.699213      19.10
 C      -2.991697     0.395187    -0.895803      47.80
 H      -4.012555     0.586316    -1.212875      22.57
 C      -2.259770     1.545207    -0.449630       9.51
 O      -2.756087     2.770229    -0.363278     116.15
 C      -4.089211     3.207411    -1.176260      78.02
 H      -5.087952     2.762211    -0.811474      23.77
 H      -4.147753     4.397215    -1.050682      23.52
 H      -4.026800     3.219404    -2.505456      22.05
 C      -0.869581     1.422202    -0.057025       2.27
 O      -0.116153     2.497933     0.522111     102.71
 C      -0.212044     0.171225    -0.036943      51.55
 H       0.617813     0.006762     0.495635      22.59
 C      -2.293096    -0.887148    -0.802354     -21.98
 C      -3.050375    -2.141136    -1.084271      98.02
 H      -4.000700    -1.973597    -1.530591      21.31
 O      -2.425481    -3.142803    -1.984651     249.27
 H      -2.900291    -3.984289    -1.951926      21.28
 C      -3.482688    -2.835914     0.252490      62.85
 H      -2.420139    -3.281190     0.594208      20.51
 O      -4.413032    -1.770156     0.904491     259.31
 H      -4.527237    -1.979036     1.926009      25.88
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 C      -4.620974    -4.005302    -0.052788      90.55
 O      -4.311808    -5.093484    -1.030072     317.87
 H      -3.369471    -5.359576    -0.856228      28.17
 H      -5.670201    -3.560885    -0.436376      24.05
 H      -4.945626    -4.725012     0.801298      24.19
55
name = lig-etoh-frame_834
 C       2.470350     2.276891    -2.143284      55.21
 H       2.088719     2.769036    -3.027802      19.53
 C       3.339751     1.451477     0.071929      49.03
 H       3.324008     1.601810     1.126123      19.37
 C       3.868349     0.262141    -0.403899       3.94
 O       4.742951    -0.623033     0.388709     247.11
 C       5.572132     0.138091     1.279986     106.38
 H       5.154735     1.162559     1.656110      24.83
 H       6.504269     0.303340     0.760059      26.85
 H       5.651639    -0.371889     2.350405      26.36
 C       3.605405    -0.035708    -1.756674      11.49
 O       4.138379    -1.190739    -2.263822     148.70
 H       4.871612    -1.708279    -1.601886      19.65
 C       2.939385     0.959204    -2.487042      67.19
 H       2.990220     0.645994    -3.477092      24.62
 C       2.613897     2.521906    -0.703594      93.30
 C       1.952344     3.655598    -0.179486     106.87
 H       2.224939     4.661032    -0.885101      20.84
 O       2.017613     3.951472     1.228754     334.36
 H       2.868786     3.771233     1.601534      29.91
 C       0.344407     3.581199    -0.462769      59.69
 H       0.321865     3.487277    -1.587591      20.30
 C      -0.211702     4.921239    -0.172398     110.61
 O       0.498520     5.987035    -0.895217     208.21
 H       0.362186     5.802508    -1.884731      28.61
 H       0.013087     5.041159     0.886433      25.70
 H      -1.279072     5.011196    -0.364242      25.73
 C      -0.847176    -1.070096    -0.336745      27.26
 H      -0.440842    -1.968915    -0.646744      18.49
 C      -3.025872     0.427305    -0.892764      24.01
 H      -4.048304     0.709017    -1.217660      18.79
 C      -2.196944     1.592335    -0.472106       1.80
 O      -2.819769     2.833909    -0.364144     170.88
 C      -4.030352     3.203572    -1.183387     124.24
 H      -4.924446     2.870763    -0.620353      24.93
 H      -4.328380     4.123223    -0.689340      23.43
 H      -3.873542     2.733744    -2.029526      26.28
 C      -0.888897     1.363974    -0.022158      24.41
 O      -0.090693     2.545606     0.528301      79.84
 C      -0.206668     0.181672    -0.027281      36.91
 H       0.927300     0.329835     0.420405      18.32
 C      -2.336856    -0.973028    -0.880605     -41.18
 C      -3.112975    -2.172960    -1.135997      79.24
 H      -3.947977    -1.712543    -1.801899      20.13
 O      -2.393415    -3.107388    -1.994704     242.08
 H      -2.901436    -3.946672    -1.701881      17.46
 C      -3.530409    -2.887258     0.276351      76.52
 H      -2.664729    -3.245682     0.814591      23.26
 O      -4.402654    -1.811981     0.931476     326.89
 H      -4.574053    -1.995656     1.852465      29.51
 C      -4.617628    -4.046175    -0.027543     104.57
 O      -4.290635    -5.106142    -1.020347     346.95
 H      -3.479111    -5.567236    -0.707454      29.61
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 H      -5.265413    -3.441453    -0.566094      28.16
 H      -4.929231    -4.594891     0.840060      26.87
55
name = lig-etoh-frame_835
 C       2.440577     2.264300    -2.109620      42.34
 H       2.035903     2.912192    -2.919077      18.99
 C       3.352257     1.443784     0.092985      59.19
 H       3.146605     1.580228     1.184371      19.71
 C       3.902719     0.238274    -0.455202      12.13
 O       4.715142    -0.604397     0.427547     282.79
 C       5.586779     0.181409     1.280082     108.82
 H       5.214086     1.122726     1.578390      25.72
 H       6.687795     0.505785     1.042661      25.42
 H       5.718879    -0.492250     2.057768      27.31
 C       3.701092    -0.048783    -1.739755      21.41
 O       4.082772    -1.186520    -2.298651     185.86
 H       4.542350    -1.575265    -1.439305      19.56
 C       2.941169     0.929301    -2.518225      65.56
 H       3.016117     0.590785    -3.660110      24.09
 C       2.570325     2.447186    -0.697809      91.02
 C       1.929156     3.753226    -0.137000     116.37
 H       2.005368     4.645660    -0.683046      22.37
 O       2.003839     3.943088     1.202064     335.42
 H       2.815392     3.643209     1.624225      29.72
 C       0.473827     3.509359    -0.413270      78.14
 H       0.244657     3.368194    -1.470220      21.32
 C      -0.213326     4.918578    -0.172850      95.11
 O       0.483740     5.999835    -0.889269     179.54
 H       0.613272     5.897311    -1.959023      24.79
 H      -0.036200     5.267674     0.874806      24.34
 H      -1.332221     4.858714    -0.431280      23.94
 C      -0.940038    -1.076464    -0.402212      11.55
 H      -0.060576    -1.942254    -0.402582      19.94
 C      -2.959541     0.421738    -0.873256      45.29
 H      -3.988038     0.543669    -1.187084      20.35
 C      -2.206342     1.580951    -0.511859      -3.52
 O      -2.865801     2.910633    -0.373034     163.52
 C      -3.979581     3.170506    -1.083977     103.40
 H      -4.801598     2.476894    -0.599144      23.39
 H      -4.166729     4.284569    -0.911037      23.25
 H      -3.855794     2.418887    -2.126180      20.89
 C      -0.884289     1.401672     0.030981     -10.65
 O      -0.101715     2.570585     0.497268     134.60
 C      -0.171286     0.140277     0.008934      25.38
 H       0.838889     0.481677    -0.012535      21.11
 C      -2.311684    -0.935862    -0.903362      -4.71
 C      -3.196596    -2.205676    -1.194906      76.29
 H      -3.994328    -1.795982    -1.769356      23.44
 O      -2.366762    -3.081426    -1.984941     236.04
 H      -2.817048    -4.054200    -1.703352      14.87
 C      -3.650686    -2.913532     0.270696      64.80
 H      -2.812650    -3.125592     1.097146      19.50
 O      -4.370923    -1.874698     0.930830     286.49
 H      -4.569114    -2.211773     2.009475      23.81
 C      -4.581010    -4.083395    -0.023219      69.94
 O      -4.246669    -5.106718    -1.006193     291.08
 H      -3.715715    -5.951739    -0.626978      26.61
 H      -5.288197    -3.361661    -0.593157      26.30
 H      -5.062103    -4.279494     1.081964      27.15
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name = lig-etoh-frame_836
 C       2.460602     2.146427    -2.078617      29.67
 H       1.999588     3.032156    -2.577902      18.00
 C       3.299105     1.484765     0.095763      79.46
 H       3.208811     1.508603     1.199938      21.44
 C       3.951175     0.272140    -0.394086      24.52
 O       4.678299    -0.561596     0.430067     244.77
 C       5.640228     0.221090     1.305400      90.69
 H       5.068924     1.151127     1.616235      25.34
 H       6.617528     0.463574     0.947751      27.26
 H       5.821693    -0.658143     2.080993      25.63
 C       3.729588     0.005673    -1.781459      32.41
 O       4.039021    -1.219150    -2.333027     179.27
 H       4.452948    -1.720587    -1.643540      24.07
 C       2.959024     0.915256    -2.589034      60.91
 H       2.848262     0.742079    -3.677156      25.23
 C       2.584267     2.363502    -0.698529      50.73
 C       1.907832     3.768864    -0.129677     116.24
 H       2.266542     4.845732    -0.705725      19.22
 O       1.996842     3.946908     1.241981     286.94
 H       2.993926     3.597605     1.506880      24.83
 C       0.533730     3.499287    -0.381300      71.06
 H       0.211712     2.999892    -1.365466      18.45
 C      -0.220721     4.931186    -0.171910     105.51
 O       0.471390     6.014378    -0.901978     217.84
 H       0.563919     5.826167    -1.793322      31.11
 H      -0.237793     5.362583     0.826102      24.64
 H      -1.218937     4.759841    -0.463614      24.93
 C      -0.972662    -1.032718    -0.473544      35.25
 H      -0.400708    -1.833248    -0.265669      25.05
 C      -2.844758     0.381648    -0.859377      64.65
 H      -3.904774     0.290859    -1.137656      22.45
 C      -2.245378     1.582054    -0.513864      -3.98
 O      -2.811214     2.945658    -0.361244     195.76
 C      -4.000770     3.068651    -1.019412     143.04
 H      -4.772841     2.412335    -0.676911      26.44
 H      -4.069318     4.100891    -1.496890      23.87
 H      -3.999859     2.892422    -2.052012      26.95
 C      -0.858140     1.468487     0.068197     -17.63
 O      -0.139630     2.555614     0.471983     161.00
 C      -0.223493     0.130963     0.009406       2.26
 H       0.938718     0.178305    -0.227405      21.52
 C      -2.273901    -0.875088    -0.884253      32.17
 C      -3.223877    -2.210942    -1.200983      65.24
 H      -4.262750    -2.062251    -1.698483      23.27
 O      -2.361117    -3.090511    -1.957979     288.57
 H      -2.569233    -3.954094    -1.950144      25.37
 C      -3.718482    -2.910656     0.253415      94.74
 H      -2.843640    -3.094677     0.880937      24.52
 O      -4.369211    -1.942002     0.956572     381.47
 H      -4.444872    -2.213946     1.796406      31.05
 C      -4.594925    -4.075482    -0.016588     112.83
 O      -4.200041    -5.118431    -0.972953     332.29
 H      -3.953025    -5.950280    -0.619227      31.90
 H      -5.526220    -3.716978    -0.467050      28.85
 H      -5.085503    -4.284923     0.883327      30.24
55
name = lig-etoh-frame_837
 C       2.494813     2.022564    -2.039088      51.55
 H       2.014118     2.852830    -2.502564      22.20
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 C       3.257884     1.480868     0.125464      55.50
 H       3.333060     1.595661     1.195464      23.05
 C       3.963134     0.370086    -0.350059      43.76
 O       4.660722    -0.506750     0.423913     218.01
 C       5.674674     0.213876     1.356236      99.59
 H       5.118267     1.039592     1.823544      27.64
 H       6.507927     0.428961     0.569357      24.41
 H       5.892324    -0.417042     2.148484      28.71
 C       3.730088     0.061129    -1.823057      41.31
 O       3.991595    -1.250742    -2.376288      85.33
 H       4.643743    -2.045556    -1.863581      20.22
 C       2.981864     0.924641    -2.666349      48.67
 H       2.732599     0.767867    -3.735047      23.04
 C       2.615070     2.345124    -0.685784      38.33
 C       1.972333     3.720111    -0.162935     114.98
 H       2.447210     4.495160    -0.654181      22.81
 O       2.031633     3.942001     1.325230     332.16
 H       2.952981     3.838710     1.391994      29.68
 C       0.455552     3.539929    -0.396132      58.58
 H       0.408507     3.067606    -1.341388      19.67
 C      -0.220613     4.943922    -0.191575      99.85
 O       0.449853     6.024485    -0.899947     213.08
 H       0.406283     5.669118    -1.954026      23.45
 H      -0.384141     5.225729     0.885361      23.23
 H      -1.290923     4.763523    -0.637679      21.42
 C      -0.955758    -0.941294    -0.507397      27.55
 H      -0.717117    -2.159651    -0.334484      21.86
 C      -2.797022     0.367000    -0.866861      62.31
 H      -3.849767     0.284023    -1.106956      25.38
 C      -2.212488     1.616576    -0.442259       4.04
 O      -2.706069     2.925151    -0.348887     152.85
 C      -4.063478     3.000134    -1.040641     105.77
 H      -5.013139     2.590661    -0.565053      25.16
 H      -4.285787     4.055127    -1.351463      25.19
 H      -3.913561     2.790905    -2.267969      23.02
 C      -0.851098     1.480149     0.044631      15.51
 O      -0.171740     2.537056     0.502010     184.26
 C      -0.291727     0.178957    -0.039068      44.64
 H       0.719298    -0.297699    -0.012596      21.71
 C      -2.278798    -0.892460    -0.866051       8.73
 C      -3.228365    -2.213607    -1.153491      86.97
 H      -4.186530    -2.203465    -1.651065      22.93
 O      -2.346147    -3.075008    -1.931043     223.95
 H      -2.598658    -4.134013    -2.094981      19.23
 C      -3.699231    -2.892622     0.177330      79.69
 H      -2.618697    -3.336941     0.574131      21.44
 O      -4.407549    -1.966456     0.974549     289.51
 H      -4.385988    -2.232861     2.071535      24.25
 C      -4.677203    -4.083674    -0.036105      96.60
 O      -4.169469    -5.113194    -0.940354     287.97
 H      -3.930213    -5.930858    -0.446339      28.99
 H      -5.704315    -3.883067    -0.463169      26.15
 H      -4.983100    -4.753659     0.978528      25.54
55
name = lig-etoh-frame_838
 C       2.501180     1.984346    -1.998434      70.77
 H       1.959259     2.616157    -2.801635      23.59
 C       3.258499     1.447749     0.209646      35.68
 H       3.428095     1.833919     1.266744      21.39
 C       3.944170     0.454237    -0.402769      27.15
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 O       4.662604    -0.455770     0.440344     232.11
 C       5.680997     0.199194     1.359671     110.52
 H       5.332523     1.088557     1.921046      25.68
 H       6.352286     0.510400     0.607233      26.32
 H       6.107611    -0.446439     2.250385      25.53
 C       3.749057     0.050093    -1.828055      19.23
 O       3.952898    -1.286129    -2.416201     210.10
 H       4.685573    -1.680528    -2.040250      27.98
 C       3.030888     0.904088    -2.723203      25.98
 H       2.679628     0.640102    -3.829259      22.32
 C       2.629741     2.372467    -0.663168      48.25
 C       2.014427     3.587156    -0.148357      83.54
 H       2.669454     4.463148    -0.814023      19.12
 O       2.088850     3.930283     1.380001     259.99
 H       3.098016     4.161380     1.547024      25.09
 C       0.375329     3.607001    -0.418991      52.89
 H       0.395283     3.351874    -1.554693      19.02
 C      -0.272690     4.940801    -0.232766     117.36
 O       0.422209     6.006549    -0.917746     268.38
 H       0.341148     5.848433    -1.875410      28.96
 H      -0.363304     5.042658     0.838214      25.13
 H      -1.212919     4.931871    -0.671241      25.20
 C      -0.960329    -0.951660    -0.518997      61.63
 H      -0.680748    -1.930975    -0.523501      26.13
 C      -2.840022     0.419367    -0.879656      41.72
 H      -3.901923     0.574207    -1.115412      24.67
 C      -2.137904     1.613317    -0.354496      18.82
 O      -2.653350     2.880100    -0.364248     116.22
 C      -4.114205     2.979911    -1.133670      95.88
 H      -4.943546     2.673606    -0.454299      25.86
 H      -4.388485     4.077479    -0.781113      22.39
 H      -3.912178     2.309713    -1.893452      24.70
 C      -0.859559     1.452325    -0.021107      28.66
 O      -0.174135     2.553446     0.567197     133.27
 C      -0.313429     0.189304    -0.092211      59.99
 H       0.644719    -0.135552     0.442798      23.45
 C      -2.332559    -0.943059    -0.862771     -20.97
 C      -3.206266    -2.216228    -1.100131      96.72
 H      -4.066476    -1.923717    -1.805151      20.92
 O      -2.315854    -3.074995    -1.911758     238.99
 H      -2.880808    -3.921664    -1.947880      21.07
 C      -3.648462    -2.907870     0.121534      89.86
 H      -2.793934    -3.501588     0.366547      22.10
 O      -4.445757    -1.979622     1.023260     314.58
 H      -4.270482    -2.185083     1.986724      26.97
 C      -4.778389    -4.160736    -0.033301      91.25
 O      -4.151822    -5.108005    -0.925491     290.90
 H      -3.681330    -5.803986    -0.298262      26.33
 H      -5.743942    -3.739283    -0.404425      27.32
 H      -4.715948    -4.691394     0.840198      27.92
55
name = lig-etoh-frame_839
 C       2.475634     2.007574    -2.042463      72.80
 H       1.906174     2.501382    -2.767810      25.44
 C       3.267682     1.483785     0.283593      20.38
 H       3.488331     1.839758     1.240553      22.05
 C       3.952029     0.444239    -0.473312      13.57
 O       4.671523    -0.412976     0.470953     234.97
 C       5.669542     0.190012     1.358410     117.69
 H       5.430644     1.154596     1.908539      24.64
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 H       6.574345     0.660838     0.766140      26.30
 H       6.191579    -0.594784     1.890952      26.20
 C       3.760376    -0.004288    -1.849772      21.17
 O       3.916678    -1.280759    -2.438078     178.44
 H       4.889919    -1.510631    -2.005287      22.88
 C       3.086423     0.860995    -2.709461      22.50
 H       2.821960     0.569444    -3.659005      23.62
 C       2.640062     2.344918    -0.629836      37.93
 C       2.015136     3.542492    -0.107597      96.29
 H       2.423356     4.307937    -0.618765      21.99
 O       2.176640     3.900056     1.392748     256.96
 H       2.993390     4.510714     1.646235      25.33
 C       0.374177     3.639001    -0.459951      55.72
 H       0.123099     3.453074    -1.477459      21.00
 C      -0.337666     4.943902    -0.269249      97.08
 O       0.403302     5.997242    -0.913289     233.98
 H       0.359114     5.946804    -1.973499      24.96
 H      -0.302541     5.151820     0.841506      23.22
 H      -1.442972     4.994840    -0.664079      22.83
 C      -1.014124    -0.996108    -0.540647      18.30
 H      -0.210834    -1.977856    -0.562990      20.67
 C      -2.912658     0.474091    -0.871967      59.65
 H      -3.927205     0.783489    -1.104060      23.50
 C      -2.155418     1.560203    -0.339424      10.25
 O      -2.659737     2.841299    -0.402932     112.22
 C      -4.129120     2.988177    -1.120797      94.56
 H      -4.749007     2.360124    -0.374292      25.52
 H      -4.194553     4.022320    -0.881377      24.39
 H      -4.113240     2.102777    -1.897392      22.30
 C      -0.800269     1.444999    -0.053537      -4.54
 O      -0.164060     2.584558     0.606313      93.79
 C      -0.255246     0.150197    -0.108885      17.63
 H       0.497570     0.415605     0.731421      18.41
 C      -2.401930    -0.914329    -0.852976       4.65
 C      -3.167233    -2.164338    -1.119000      98.98
 H      -3.860279    -1.648976    -1.790415      21.60
 O      -2.308542    -3.085396    -1.880732     250.79
 H      -2.943101    -3.816774    -1.864001      21.83
 C      -3.703314    -2.957555     0.117359      69.63
 H      -2.767855    -3.539787     0.627967      19.50
 O      -4.449067    -1.999109     1.048664     315.57
 H      -4.190340    -2.208373     2.029935      24.57
 C      -4.807871    -4.190924    -0.052034      71.13
 O      -4.145737    -5.124014    -0.928088     338.18
 H      -3.413696    -5.571158    -0.512501      28.95
 H      -5.748207    -3.728827    -0.302155      27.90
 H      -4.731343    -4.493410     1.160699      26.58
55
name = lig-etoh-frame_840
 C       2.472962     2.014035    -2.103801      73.95
 H       1.729606     2.724693    -2.641336      22.32
 C       3.313681     1.512894     0.243088      11.93
 H       3.557667     1.725748     1.343953      21.35
 C       3.977891     0.384967    -0.465352      24.20
 O       4.689273    -0.380551     0.487014     233.41
 C       5.700868     0.214991     1.309946     120.29
 H       5.278365     0.948138     1.999013      26.31
 H       6.595070     0.636896     0.897711      28.13
 H       6.082128    -0.784078     1.732300      24.81
 C       3.751959    -0.053629    -1.852610      28.08
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 O       3.929644    -1.266899    -2.423483     159.66
 H       4.842807    -1.725782    -2.102407      24.24
 C       3.107730     0.874247    -2.613130      42.79
 H       2.948335     0.481079    -3.773497      21.57
 C       2.623247     2.285298    -0.624874      27.98
 C       1.948098     3.580573    -0.037515      99.03
 H       2.328142     4.653624    -0.631916      18.88
 O       2.250136     3.858808     1.385574     290.38
 H       2.859220     4.534607     1.380047      29.43
 C       0.404997     3.625094    -0.455418      55.96
 H       0.010113     3.159385    -1.442077      19.25
 C      -0.409864     4.980116    -0.272159     106.68
 O       0.390377     6.005011    -0.916134     226.66
 H       0.415780     5.861361    -1.963565      25.51
 H      -0.341639     5.372764     0.730454      23.96
 H      -1.420194     4.854538    -0.523745      25.37
 C      -1.012572    -1.049434    -0.539947      26.85
 H      -0.288691    -1.792440    -0.580693      23.04
 C      -2.971583     0.485105    -0.835466      71.16
 H      -4.015391     0.623817    -1.090422      24.33
 C      -2.212496     1.515628    -0.393873       3.31
 O      -2.705654     2.812876    -0.470104     158.63
 C      -4.089087     2.917500    -1.031832     108.55
 H      -4.640313     2.314105    -0.311969      25.49
 H      -4.195815     4.075486    -1.333244      23.59
 H      -4.310228     2.680653    -2.135835      25.41
 C      -0.744828     1.450021    -0.056281     -14.17
 O      -0.159648     2.605374     0.595320     124.36
 C      -0.195686     0.161619    -0.073671       9.79
 H       0.641538     0.282397     0.598062      20.26
 C      -2.408505    -0.829870    -0.817741      13.25
 C      -3.132354    -2.095918    -1.161849      79.23
 H      -4.012861    -1.764172    -1.802272      22.35
 O      -2.316946    -3.089872    -1.842209     175.79
 H      -2.922846    -4.036276    -1.939303      16.39
 C      -3.805872    -2.998919     0.168358      80.18
 H      -2.953177    -3.209109     0.802343      21.05
 O      -4.429017    -2.029054     1.040631     343.46
 H      -4.196430    -2.246143     2.112008      23.10
 C      -4.735656    -4.167033    -0.007922      90.57
 O      -4.167556    -5.151880    -0.950447     317.53
 H      -3.195143    -5.415865    -0.727969      26.08
 H      -5.814654    -3.931890    -0.385464      25.75
 H      -5.018646    -4.398520     0.955528      29.70
55
name = lig-etoh-frame_841
 C       2.468498     2.040586    -2.097289      19.51
 H       1.846110     2.762128    -2.558157      19.35
 C       3.412026     1.487462     0.134782      49.36
 H       3.500337     1.609001     1.184400      20.56
 C       3.996006     0.326241    -0.402093      30.55
 O       4.713455    -0.374411     0.463533     256.16
 C       5.742321     0.210004     1.285286     102.79
 H       5.174748     0.646728     2.185373      25.62
 H       6.586628     0.722442     0.725544      26.40
 H       5.966125    -0.726830     1.844560      25.86
 C       3.754827    -0.070099    -1.762847      30.91
 O       3.974511    -1.289557    -2.408957     191.15
 H       4.646356    -1.846770    -2.085116      27.53
 C       3.075457     0.910921    -2.589029      47.69
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 H       3.058962     0.657696    -3.537362      26.07
 C       2.558512     2.296730    -0.663921      85.66
 C       1.883762     3.682657    -0.033531     118.39
 H       2.240146     4.474810    -0.506634      27.17
 O       2.288060     3.799774     1.362680     263.57
 H       2.957221     4.558583     1.117915      26.86
 C       0.397804     3.583339    -0.389563      71.31
 H       0.315891     3.020200    -1.298559      20.90
 C      -0.415439     5.008540    -0.253514      97.87
 O       0.370809     6.020221    -0.947880     257.55
 H       0.435123     5.790883    -1.870638      29.77
 H      -0.461620     5.415641     0.798596      23.88
 H      -1.502979     4.748193    -0.586825      23.00
 C      -0.982013    -0.982363    -0.501003     -11.35
 H      -0.488844    -2.127878    -0.634253      22.24
 C      -3.028134     0.430945    -0.788028      64.42
 H      -4.064237     0.379301    -1.093875      22.47
 C      -2.211114     1.530176    -0.466903       3.11
 O      -2.763133     2.794982    -0.562253     197.76
 C      -4.032326     2.891776    -0.975316     140.64
 H      -4.866252     2.535145    -0.297748      26.76
 H      -4.339832     3.908568    -1.209216      26.15
 H      -4.233498     2.864052    -2.130835      24.56
 C      -0.764472     1.455364    -0.039924      -3.50
 O      -0.169341     2.605218     0.553549     170.59
 C      -0.171116     0.183424    -0.022186      15.57
 H       0.951994    -0.277867     0.173494      21.17
 C      -2.346974    -0.797370    -0.781851      16.03
 C      -3.172782    -2.075474    -1.192466      78.15
 H      -4.106800    -2.077015    -1.765303      22.43
 O      -2.327154    -3.103703    -1.811367     262.18
 H      -2.792926    -3.843560    -1.960035      25.49
 C      -3.873105    -2.944613     0.236944      65.04
 H      -2.864271    -3.240723     0.775256      20.72
 O      -4.429999    -2.040821     1.028220     337.62
 H      -4.354439    -2.264906     2.020446      25.48
 C      -4.678619    -4.139963    -0.004583     101.11
 O      -4.194485    -5.183809    -0.970692     303.21
 H      -3.203206    -5.386656    -0.809773      25.77
 H      -5.559880    -4.014979    -0.593496      24.45
 H      -5.188180    -4.704738     0.979841      25.49
55
name = lig-etoh-frame_842
 C       2.459509     2.090640    -2.020053      55.19
 H       1.984723     2.775919    -2.820859      20.51
 C       3.467218     1.486658    -0.005194      81.27
 H       3.486510     1.657845     1.095031      20.88
 C       3.994119     0.295688    -0.368710      31.93
 O       4.766311    -0.428686     0.436469     289.75
 C       5.752460     0.171374     1.313612     109.06
 H       5.341104     0.737222     2.113662      28.43
 H       6.402140     0.834444     0.722115      26.86
 H       6.272871    -0.664312     1.862000      26.71
 C       3.746250    -0.058849    -1.675053      30.82
 O       4.011785    -1.305184    -2.403238      98.27
 H       4.671940    -1.985304    -1.717231      19.61
 C       3.053184     0.914299    -2.550604      66.08
 H       3.083953     0.764764    -3.783233      24.34
 C       2.510311     2.352395    -0.695027      76.42
 C       1.839922     3.691035    -0.053955     102.82
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 H       2.378924     4.639661    -0.731083      20.74
 O       2.310760     3.765505     1.321524     238.09
 H       3.186604     4.345071     1.339943      27.10
 C       0.369998     3.563868    -0.280382      77.39
 H       0.538622     3.216203    -1.372500      20.13
 C      -0.396874     4.997430    -0.237836     109.03
 O       0.336268     6.036566    -0.974915     235.64
 H       0.448679     5.713526    -2.042955      23.40
 H      -0.551211     5.251399     0.806307      25.26
 H      -1.336485     4.878360    -0.737318      24.56
 C      -0.924492    -0.898754    -0.446417      50.24
 H      -0.922209    -1.959541    -0.567047      23.16
 C      -3.033325     0.358757    -0.733893      46.17
 H      -4.071901     0.355066    -1.066548      20.47
 C      -2.190789     1.550979    -0.533786       7.69
 O      -2.765996     2.789051    -0.633804     185.37
 C      -4.078396     2.920833    -0.982682     116.10
 H      -4.993881     2.620586    -0.420485      24.74
 H      -4.312486     4.130412    -0.661420      22.14
 H      -4.076917     2.346011    -1.948275      23.37
 C      -0.826910     1.454411    -0.012593       5.76
 O      -0.197340     2.585136     0.514694     190.55
 C      -0.140416     0.123903    -0.000073      57.26
 H       0.787082    -0.220588    -0.246707      22.69
 C      -2.309954    -0.843152    -0.773311       6.98
 C      -3.237675    -2.127498    -1.168670      70.08
 H      -4.123745    -1.991900    -1.824674      23.74
 O      -2.310787    -3.082546    -1.781505     202.02
 H      -2.968489    -3.916021    -1.994284      18.74
 C      -3.795893    -2.878054     0.283577      72.07
 H      -2.854445    -3.411489     0.500710      23.39
 O      -4.481492    -1.992733     1.032521     295.18
 H      -4.564470    -2.332899     2.089287      23.94
 C      -4.696557    -4.193461    -0.032967      96.55
 O      -4.200758    -5.204133    -0.986790     333.58
 H      -3.361631    -5.601596    -0.734948      29.20
 H      -5.519615    -3.715181    -0.726060      25.41
 H      -4.928825    -4.741286     0.775998      29.58
55
name = lig-etoh-frame_843
 C       2.442625     2.127428    -2.031175      62.47
 H       2.186385     2.693445    -2.918283      19.94
 C       3.441944     1.567192    -0.068166      76.80
 H       3.591849     1.839442     0.996875      18.77
 C       3.993720     0.286449    -0.372017      20.77
 O       4.844379    -0.534462     0.435780     264.27
 C       5.756509     0.131755     1.355361     117.22
 H       5.371913     0.959630     2.064073      26.35
 H       6.321814     0.902217     0.773570      28.26
 H       6.646520    -0.530485     1.629194      26.27
 C       3.704418    -0.070087    -1.715922      21.25
 O       4.062463    -1.315873    -2.345370     184.56
 H       4.561501    -1.711192    -1.725041      26.84
 C       3.050535     0.890905    -2.520364      37.72
 H       3.052481     0.819572    -3.517633      25.62
 C       2.515208     2.418417    -0.673952      68.31
 C       1.904405     3.671460    -0.090602     111.74
 H       2.142553     4.437139    -0.647209      26.14
 O       2.331920     3.753701     1.292618     316.02
 H       3.212838     3.950998     1.492437      31.70
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 C       0.357152     3.604818    -0.239965      85.42
 H       0.306327     3.537593    -1.329495      21.28
 C      -0.360443     4.958620    -0.247732     106.37
 O       0.304625     6.038198    -1.008839     282.96
 H       0.366088     5.809543    -1.898463      31.92
 H      -0.565177     5.245655     0.814664      24.20
 H      -1.318533     4.916448    -0.839166      22.60
 C      -0.972031    -0.888520    -0.411891      41.95
 H      -0.554761    -2.007702    -0.428699      22.39
 C      -2.976391     0.316461    -0.695972      53.10
 H      -4.022978     0.468739    -0.953819      21.77
 C      -2.185517     1.526900    -0.566821      14.02
 O      -2.716029     2.794103    -0.661030     159.31
 C      -4.194236     2.992401    -1.012403     115.63
 H      -4.881842     2.338141    -0.304933      24.30
 H      -4.130711     3.960188    -0.692782      24.67
 H      -4.287133     2.304079    -1.889107      22.36
 C      -0.886618     1.416379    -0.005055       2.24
 O      -0.242144     2.545859     0.502109     165.81
 C      -0.144888     0.114153    -0.011735      42.29
 H       1.045321     0.212324    -0.299267      19.89
 C      -2.350598    -0.895879    -0.773112      31.83
 C      -3.267574    -2.191201    -1.081358      84.85
 H      -3.981119    -1.694239    -1.805952      23.50
 O      -2.314665    -3.072777    -1.760565     220.26
 H      -2.943145    -3.906413    -1.973608      20.62
 C      -3.677848    -2.875252     0.235107      76.51
 H      -2.704423    -3.317361     0.651192      23.44
 O      -4.553429    -1.927144     1.076193     308.36
 H      -4.557760    -2.242134     1.921136      29.20
 C      -4.722665    -4.206282    -0.134053      82.40
 O      -4.195783    -5.213324    -1.017405     264.64
 H      -3.540419    -5.917978    -0.564290      24.66
 H      -5.565773    -3.636952    -0.427565      28.88
 H      -4.902370    -4.734668     0.970453      26.82
55
name = lig-etoh-frame_844
 C       2.456613     2.105653    -2.106451      37.86
 H       2.128888     2.832261    -2.876560      21.77
 C       3.425251     1.635919    -0.012511      55.17
 H       3.745932     2.001616     0.942087      19.46
 C       3.991153     0.304261    -0.401986      16.06
 O       4.906372    -0.634426     0.438133     207.17
 C       5.798069     0.154607     1.360107     114.60
 H       5.248959     0.658701     2.154896      27.19
 H       6.269965     0.919737     0.694879      28.61
 H       6.618703    -0.459187     1.598425      27.85
 C       3.667361    -0.115525    -1.786923      12.21
 O       4.083262    -1.283309    -2.284485     112.61
 H       4.851204    -1.754122    -1.581928      19.39
 C       3.028640     0.899421    -2.465910      40.97
 H       3.002598     0.678051    -3.654030      20.51
 C       2.553760     2.468057    -0.696875      39.45
 C       1.980143     3.614041    -0.080018     104.32
 H       2.132985     4.707045    -0.769503      16.88
 O       2.322421     3.758159     1.286402     266.86
 H       3.398136     3.603484     1.387024      23.08
 C       0.367412     3.657900    -0.271254      50.92
 H       0.073810     3.412794    -1.353266      18.89
 C      -0.357353     4.954035    -0.249362     106.14
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 O       0.283330     6.039829    -0.994290     234.17
 H       0.307113     5.805103    -2.111630      21.70
 H      -0.533795     5.449318     0.716408      24.09
 H      -1.354007     4.706351    -0.689789      23.07
 C      -1.018135    -1.024487    -0.395892      33.13
 H      -0.114782    -1.658179    -0.340801      21.00
 C      -2.920886     0.336455    -0.692781      66.29
 H      -3.997528     0.491252    -0.816247      22.29
 C      -2.195622     1.478532    -0.557332      17.26
 O      -2.673329     2.801799    -0.683148      95.16
 C      -4.273798     2.969916    -1.001538      89.02
 H      -4.536561     2.330043    -0.178661      22.65
 H      -4.337075     4.184363    -1.030772      22.96
 H      -4.696016     2.826699    -2.135468      22.66
 C      -0.905150     1.361153    -0.021426      10.14
 O      -0.288218     2.515407     0.510752     129.29
 C      -0.161725     0.208863    -0.061994      19.80
 H       0.826131     0.469126     0.113619      20.32
 C      -2.398988    -0.965998    -0.742120      37.57
 C      -3.218329    -2.188808    -0.987428     105.80
 H      -3.967879    -1.744064    -1.621025      24.48
 O      -2.341979    -3.081235    -1.752879     271.86
 H      -2.727708    -3.884367    -1.911232      26.40
 C      -3.624325    -2.909890     0.181714      82.08
 H      -2.807448    -2.973432     0.959234      21.31
 O      -4.599334    -1.880189     1.072263     194.78
 H      -4.403208    -2.249790     2.138990      22.82
 C      -4.694736    -4.196593    -0.149744      95.93
 O      -4.199147    -5.222149    -1.060140     269.53
 H      -3.807714    -5.915867    -0.502465      28.55
 H      -5.772138    -3.772276    -0.340535      28.34
 H      -4.921794    -4.488613     0.793287      30.88
55
name = lig-etoh-frame_845
 C       2.477739     2.100203    -2.147219      31.13
 H       1.957975     2.883666    -2.766806      21.06
 C       3.457155     1.627365     0.089642      96.13
 H       3.927349     2.050242     1.040455      22.49
 C       3.981543     0.337388    -0.440681       6.67
 O       4.937612    -0.685721     0.422690     177.14
 C       5.825365     0.190781     1.314910     102.41
 H       5.183928     0.274307     2.275453      24.04
 H       6.196308     1.026477     0.742638      28.53
 H       6.583946    -0.584175     1.809860      25.18
 C       3.661918    -0.126487    -1.734621       7.76
 O       4.109827    -1.275287    -2.225457     174.83
 H       4.963503    -1.655542    -1.845370      22.76
 C       2.988427     0.892185    -2.534855      52.29
 H       2.896515     0.539192    -3.537665      21.70
 C       2.633153     2.456906    -0.797256      38.54
 C       1.988757     3.657480    -0.092266     115.27
 H       2.297949     4.478931    -0.532164      23.49
 O       2.325192     3.768792     1.298744     339.11
 H       3.255107     3.525594     1.203509      28.10
 C       0.395254     3.638293    -0.348517      42.58
 H       0.221150     3.111739    -1.294092      19.60
 C      -0.390618     5.001168    -0.228016     106.67
 O       0.263487     6.029647    -1.002758     287.56
 H       0.328155     5.815793    -1.920329      29.78
 H      -0.458773     5.533851     0.731899      23.89
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 H      -1.387900     4.608353    -0.503621      23.16
 C      -0.954585    -1.110743    -0.367152      22.38
 H      -0.189120    -1.885141    -0.428417      20.75
 C      -2.928971     0.342344    -0.720717      64.28
 H      -4.002827     0.392181    -0.789569      23.27
 C      -2.213411     1.475165    -0.525725      16.11
 O      -2.669381     2.807077    -0.730459      92.28
 C      -4.284723     2.987349    -1.008211     104.61
 H      -4.667979     2.491111    -0.097150      24.38
 H      -4.625333     4.008500    -1.037480      26.07
 H      -4.768772     2.959455    -1.992321      24.41
 C      -0.895822     1.387043    -0.051961      29.05
 O      -0.324112     2.515720     0.538260     125.95
 C      -0.265203     0.261989    -0.122327      14.80
 H       0.768661     0.305157     0.535076      19.42
 C      -2.362909    -1.014982    -0.664781      22.70
 C      -3.141871    -2.162696    -0.956159      98.08
 H      -4.194941    -2.040458    -1.453991      22.69
 O      -2.352536    -3.075567    -1.761207     190.68
 H      -2.711620    -4.158113    -1.769644      17.16
 C      -3.683804    -2.943467     0.221373      84.22
 H      -2.966059    -2.966848     1.009156      22.46
 O      -4.617615    -1.879259     1.064148     287.44
 H      -4.296075    -1.998850     1.943364      27.61
 C      -4.647359    -4.132509    -0.135710      96.26
 O      -4.228901    -5.216026    -1.096227     245.40
 H      -3.861061    -5.895433    -0.546510      29.90
 H      -5.583333    -3.909817    -0.593628      27.34
 H      -4.873886    -4.609660     0.972055      26.28
55
name = lig-etoh-frame_846
 C       2.487007     2.119780    -2.157211      38.30
 H       1.863529     2.708221    -2.785866      21.71
 C       3.516399     1.574525     0.141643      70.71
 H       3.912298     1.888819     1.052263      23.38
 C       3.994930     0.370648    -0.405854       7.35
 O       4.948207    -0.667613     0.377207     204.57
 C       5.815838     0.148566     1.296872     121.61
 H       5.211852     0.282032     2.199388      26.81
 H       6.166999     1.191936     0.990623      28.59
 H       6.569226    -0.464449     1.653943      27.66
 C       3.657385    -0.060643    -1.646032      16.70
 O       4.123798    -1.286808    -2.208325     188.16
 H       5.027125    -1.604404    -1.830021      24.00
 C       2.960602     0.816643    -2.639496      49.04
 H       2.746784     0.448916    -3.699042      20.69
 C       2.751329     2.418220    -0.826769      47.45
 C       1.943844     3.685840    -0.113684     115.12
 H       2.574339     4.705992    -0.590821      19.17
 O       2.315275     3.774625     1.308811     318.81
 H       3.283547     3.703048     1.335468      27.86
 C       0.429217     3.575335    -0.400725      42.05
 H       0.416792     3.112148    -1.400580      18.65
 C      -0.410963     5.031611    -0.204878      92.97
 O       0.237236     6.025245    -0.998660     257.47
 H       0.348775     5.710752    -2.035370      24.32
 H      -0.321286     5.334909     0.879618      23.14
 H      -1.505719     4.803909    -0.446882      22.25
 C      -0.865144    -1.103212    -0.347416      45.84
 H      -0.599974    -2.243333    -0.496796      19.28
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 C      -2.964761     0.282601    -0.750231      47.19
 H      -4.053752     0.287129    -0.920921      23.19
 C      -2.257888     1.527350    -0.506339       2.36
 O      -2.723678     2.815834    -0.797241     135.07
 C      -4.252186     3.015034    -0.979712      95.24
 H      -5.026213     2.610508    -0.225633      24.69
 H      -4.528304     4.159233    -0.672863      22.80
 H      -4.593131     2.378271    -1.983043      22.10
 C      -0.906763     1.516458    -0.089685       7.00
 O      -0.336639     2.553376     0.575586     142.29
 C      -0.308116     0.156246    -0.132814      22.74
 H       0.452015    -0.038934     0.560043      21.82
 C      -2.254324    -0.984132    -0.575033      -0.05
 C      -3.144961    -2.211844    -0.959405      85.42
 H      -4.091693    -2.046667    -1.408788      23.80
 O      -2.348397    -3.103537    -1.788387     262.08
 H      -2.728505    -3.915944    -1.506532      22.60
 C      -3.787658    -2.927652     0.323550      82.23
 H      -2.934162    -3.406218     1.012086      21.21
 O      -4.623338    -1.903177     1.007889     338.25
 H      -4.238373    -1.867195     1.998776      25.02
 C      -4.606528    -4.098558    -0.074803     101.60
 O      -4.259481    -5.192788    -1.117253     223.99
 H      -3.660081    -5.953678    -0.677115      26.91
 H      -5.436039    -3.701365    -0.743038      26.06
 H      -4.830363    -4.688656     0.745953      28.11
55
name = lig-etoh-frame_847
 C       2.521334     2.065410    -2.174097      92.12
 H       1.782203     2.616760    -2.871627      21.52
 C       3.565696     1.534796     0.118546      24.13
 H       3.769390     1.820062     1.217862      17.74
 C       4.053297     0.359988    -0.302303      16.21
 O       4.943394    -0.577777     0.307088     255.35
 C       5.769955     0.100274     1.296200     115.17
 H       5.178816     0.415972     2.224664      25.37
 H       6.101322     1.107728     1.098441      28.18
 H       6.812628    -0.475741     1.402655      25.09
 C       3.648521    -0.008956    -1.681024      22.34
 O       4.118827    -1.281912    -2.197386     147.40
 H       4.995309    -1.595604    -1.568369      20.49
 C       2.941540     0.746566    -2.685464      53.22
 H       2.638752     0.383076    -3.734188      22.44
 C       2.851241     2.407042    -0.761944      76.88
 C       1.984844     3.712145    -0.144108     110.19
 H       2.258646     4.530079    -0.609841      25.19
 O       2.284308     3.770205     1.311494     260.06
 H       3.298042     4.154422     1.527454      24.52
 C       0.437756     3.544019    -0.411300      48.95
 H       0.371132     3.284105    -1.513189      20.17
 C      -0.391980     5.003400    -0.190005     103.29
 O       0.210704     6.026689    -1.009473     273.22
 H       0.280363     5.647021    -1.960043      27.94
 H      -0.198597     5.114940     0.862467      23.83
 H      -1.389856     4.981372    -0.505260      24.40
 C      -0.864591    -1.108377    -0.367251      82.29
 H      -0.683729    -2.117658    -0.338585      22.76
 C      -2.961425     0.228743    -0.752908      52.87
 H      -3.988555     0.174344    -1.093582      22.96
 C      -2.319211     1.572924    -0.519002      -4.54
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 O      -2.831557     2.826085    -0.852062     188.78
 C      -4.230229     3.018034    -0.942421     124.58
 H      -4.954924     2.517554    -0.283243      26.72
 H      -4.152466     4.108445    -0.782609      24.56
 H      -4.324725     2.392236    -1.783628      24.63
 C      -0.926469     1.549222    -0.127311     -16.83
 O      -0.312112     2.622797     0.588490     137.76
 C      -0.304656     0.076955    -0.080987       3.75
 H       0.678482    -0.047750     0.515390      19.98
 C      -2.224423    -0.937277    -0.541232       2.47
 C      -3.145757    -2.262182    -0.926878      55.53
 H      -3.966120    -1.729056    -1.622611      21.05
 O      -2.344017    -3.129089    -1.803007     224.31
 H      -2.730074    -4.031942    -1.490671      17.30
 C      -3.803194    -2.906011     0.436175     102.30
 H      -3.073514    -3.477624     0.921931      23.10
 O      -4.610716    -1.949473     0.947911     347.66
 H      -4.388366    -1.847270     1.997562      25.08
 C      -4.634545    -4.106278    -0.071356      90.48
 O      -4.261663    -5.164944    -1.120251     278.35
 H      -3.478109    -5.714055    -0.944499      28.53
 H      -5.434013    -3.483948    -0.513259      26.53
 H      -5.075207    -4.758923     0.812788      26.14
55
name = lig-etoh-frame_848
 C       2.567945     1.968510    -2.164886      62.61
 H       1.949123     2.590603    -2.729088      21.89
 C       3.602839     1.560596     0.132228      55.71
 H       3.521786     1.841602     1.146877      20.26
 C       4.094269     0.298432    -0.304238      19.71
 O       4.939980    -0.463745     0.246684     222.46
 C       5.746710     0.065940     1.316266     103.82
 H       5.256574     0.175157     2.315379      27.94
 H       6.031015     1.080641     0.854920      25.77
 H       6.637760    -0.445955     1.342620      29.20
 C       3.678067    -0.023458    -1.761196      34.37
 O       4.114944    -1.258873    -2.160545     177.86
 H       4.685130    -1.604967    -1.580081      25.22
 C       2.920132     0.726143    -2.651503      26.01
 H       2.670187     0.318419    -3.593011      26.43
 C       2.881286     2.427311    -0.732346      81.12
 C       2.052869     3.649857    -0.141332     100.64
 H       2.112803     4.757023    -0.839945      19.96
 O       2.259652     3.786787     1.315400     303.21
 H       2.932319     4.403256     1.397835      30.88
 C       0.418841     3.568102    -0.397917      72.25
 H       0.183966     3.302442    -1.409967      22.40
 C      -0.308776     4.924713    -0.199374      98.06
 O       0.195859     6.033002    -1.015326     256.15
 H       0.217686     5.706141    -1.931219      30.02
 H      -0.185317     5.184769     0.906688      23.20
 H      -1.414148     4.842701    -0.531507      22.58
 C      -0.927596    -1.108139    -0.385101      32.01
 H      -0.291174    -2.108969    -0.115433      22.19
 C      -2.927595     0.254744    -0.740195      61.04
 H      -3.913874     0.101811    -1.202627      23.71
 C      -2.347738     1.571663    -0.554934      13.22
 O      -2.892604     2.812778    -0.862334     182.41
 C      -4.215692     3.003606    -0.914756     107.83
 H      -4.707769     2.435874    -0.026425      23.86
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 H      -4.259105     4.155648    -1.127247      23.12
 H      -4.565091     2.741572    -2.148995      22.13
 C      -0.949921     1.469615    -0.132647     -32.08
 O      -0.269814     2.682759     0.545644     107.07
 C      -0.231542     0.120561     0.032757       6.53
 H       0.895448     0.289587     0.137703      21.20
 C      -2.302413    -0.957059    -0.574969      22.00
 C      -3.128001    -2.245806    -0.890397      75.88
 H      -3.755043    -1.760177    -1.554629      23.88
 O      -2.349345    -3.158778    -1.786198     186.43
 H      -2.626942    -4.213817    -1.825119      16.95
 C      -3.750427    -2.937885     0.431250      87.22
 H      -2.873997    -3.222302     1.246899      21.71
 O      -4.614802    -1.973178     0.933386     349.52
 H      -4.584008    -1.996640     1.836554      30.32
 C      -4.730583    -4.151399    -0.067367      86.50
 O      -4.256689    -5.109119    -1.118549     277.47
 H      -3.315750    -5.450223    -1.004944      26.02
 H      -5.610714    -3.580677    -0.421015      27.54
 H      -5.256189    -4.594163     0.787764      27.86
55
name = lig-etoh-frame_849
 C       2.608325     1.934048    -2.078663      44.71
 H       2.050944     2.707137    -2.715970      21.00
 C       3.615083     1.597073     0.141301      83.10
 H       3.499225     1.894454     1.223385      21.25
 C       4.024033     0.341278    -0.448038      31.45
 O       4.978164    -0.429182     0.228770     222.73
 C       5.730336     0.083575     1.314446      94.88
 H       5.275126    -0.063895     2.321678      27.04
 H       5.969656     1.060184     0.938235      25.48
 H       6.648277    -0.651768     1.448824      26.15
 C       3.754292    -0.072729    -1.762062      28.17
 O       4.092984    -1.247553    -2.159476     154.55
 H       4.693564    -1.818828    -1.386177      17.63
 C       2.916601     0.712091    -2.575849      74.11
 H       2.660156     0.237283    -3.649342      24.54
 C       2.863506     2.432395    -0.765611      87.43
 C       2.082197     3.602161    -0.175946     117.30
 H       2.274551     4.451139    -0.612870      26.02
 O       2.221235     3.810947     1.296954     282.24
 H       2.818287     4.634208     1.319553      27.86
 C       0.419164     3.595165    -0.378891      72.22
 H       0.124600     3.170776    -1.407067      21.96
 C      -0.233247     4.869313    -0.206292     111.81
 O       0.193426     6.035472    -1.007774     234.34
 H       0.181013     5.801044    -2.093803      24.41
 H      -0.270588     5.333859     0.755062      24.21
 H      -1.226199     4.527255    -0.387940      23.45
 C      -0.925100    -1.065253    -0.330983      15.71
 H      -0.241554    -1.802052    -0.157193      25.46
 C      -2.926808     0.325063    -0.749644      52.68
 H      -3.911990     0.259361    -1.205731      23.41
 C      -2.320470     1.522326    -0.588033      26.01
 O      -2.863857     2.778102    -0.852656     205.47
 C      -4.267983     3.009633    -0.957210     125.83
 H      -4.659596     2.630528    -0.060513      26.81
 H      -4.655163     4.058517    -1.097892      25.07
 H      -4.895038     2.844301    -1.946966      23.97
 C      -0.945488     1.376589    -0.085536     -27.77
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 O      -0.245740     2.692394     0.472989      93.65
 C      -0.192574     0.232408     0.091348      38.89
 H       0.865161     0.427102    -0.062478      23.13
 C      -2.350115    -1.042567    -0.620612      20.89
 C      -3.092089    -2.245736    -0.855887      81.75
 H      -4.091318    -1.977249    -1.509242      21.31
 O      -2.330310    -3.185761    -1.769382     256.93
 H      -2.710867    -3.961895    -1.972119      25.15
 C      -3.675371    -3.000999     0.373655      92.23
 H      -2.986264    -2.954227     1.149219      23.56
 O      -4.635697    -1.971608     0.926849     251.58
 H      -4.767068    -2.242861     2.015803      26.16
 C      -4.812174    -4.175294    -0.060985      78.58
 O      -4.261091    -5.047568    -1.106298     260.09
 H      -3.290451    -5.263351    -0.802052      25.76
 H      -5.681419    -3.725102    -0.620962      26.38
 H      -5.223608    -4.699605     0.902047      26.77
55
name = lig-etoh-frame_850
 C       2.602642     1.991862    -2.009503      54.14
 H       2.151296     2.628714    -2.727448      21.64
 C       3.583879     1.627599     0.106589      45.03
 H       3.770233     1.816860     1.174248      19.63
 C       3.979071     0.453907    -0.525365      27.38
 O       5.008440    -0.450457     0.205147     227.32
 C       5.737670     0.089003     1.315140     111.82
 H       5.095068    -0.059922     2.273742      28.25
 H       6.072631     1.197683     1.368998      28.09
 H       6.569727    -0.586238     1.493850      28.67
 C       3.791809    -0.081981    -1.733119      28.00
 O       4.098573    -1.322114    -2.175527     211.99
 H       4.684620    -1.785123    -1.529574      19.16
 C       2.936193     0.667546    -2.525886      72.58
 H       2.663504     0.417176    -3.455824      28.49
 C       2.842569     2.404623    -0.759008      81.23
 C       2.048654     3.543803    -0.191039     116.19
 H       2.643144     4.618152    -0.675478      20.80
 O       2.190267     3.837061     1.262488     262.28
 H       2.773639     4.705067     1.371697      27.05
 C       0.492354     3.550698    -0.419428      83.76
 H       0.347546     3.270367    -1.430017      22.13
 C      -0.202656     4.890417    -0.216793     100.84
 O       0.193702     6.025625    -1.025349     278.13
 H       0.196227     5.803368    -1.907438      33.06
 H      -0.233084     5.363075     0.822431      23.20
 H      -1.279950     4.479672    -0.341000      22.03
 C      -0.911464    -0.941182    -0.238609      22.89
 H      -0.258395    -1.949900    -0.294788      20.72
 C      -2.969118     0.308343    -0.791510      37.97
 H      -3.996565     0.514389    -1.135707      20.14
 C      -2.246458     1.477711    -0.594683      10.36
 O      -2.809163     2.755619    -0.855160     140.56
 C      -4.355230     3.030404    -1.006281      97.60
 H      -4.932914     2.721018    -0.005953      23.48
 H      -4.578493     4.161521    -0.805331      22.71
 H      -5.042168     2.319679    -1.701484      21.57
 C      -0.927379     1.402564    -0.011462      11.47
 O      -0.253433     2.638752     0.422440     156.89
 C      -0.224556     0.296151     0.078216      60.30
 H       0.949504     0.333291    -0.008089      21.07
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 C      -2.298876    -1.046176    -0.641785       0.65
 C      -3.136483    -2.312194    -0.895316     101.72
 H      -4.116402    -2.218367    -1.224224      23.73
 O      -2.278497    -3.174390    -1.746399     221.70
 H      -3.103630    -3.869397    -2.036134      19.26
 C      -3.694252    -3.027128     0.305784      77.42
 H      -2.843019    -3.182842     1.180519      21.71
 O      -4.661381    -1.974246     0.947195     263.41
 H      -4.773196    -2.352240     1.822234      28.29
 C      -4.843875    -4.178165    -0.056841      94.48
 O      -4.254743    -5.000801    -1.077410     279.51
 H      -3.475000    -5.325123    -0.679868      30.10
 H      -5.632451    -3.714395    -0.594650      28.45
 H      -5.001320    -4.815592     0.842406      27.17
55
name = lig-etoh-frame_851
 C       2.580338     2.005627    -2.040110      37.66
 H       2.058873     2.642659    -2.791755      17.97
 C       3.564773     1.624591     0.074825       1.28
 H       4.006866     1.816552     1.026731      20.80
 C       4.063800     0.511428    -0.461082      44.31
 O       5.020768    -0.450062     0.164346     232.61
 C       5.720607     0.100222     1.356451     126.90
 H       4.981328     0.042271     2.168742      26.87
 H       6.096354     1.087117     1.582162      30.66
 H       6.649230    -0.535665     1.475992      28.14
 C       3.770622    -0.105252    -1.759357      15.03
 O       4.105919    -1.410959    -2.203284     159.36
 H       4.883596    -1.834554    -1.639455      19.19
 C       2.953753     0.702168    -2.466508      83.08
 H       2.584384     0.495315    -3.597378      26.49
 C       2.788991     2.409751    -0.683318      83.82
 C       2.036264     3.589263    -0.191852     128.36
 H       2.468964     4.294799    -0.694908      24.30
 O       2.164555     3.855929     1.234061     333.07
 H       2.764907     4.523898     1.366136      31.93
 C       0.592597     3.504890    -0.495611      45.90
 H       0.522492     3.358273    -1.634287      16.59
 C      -0.222754     4.933712    -0.207956     100.43
 O       0.197240     6.016902    -1.028208     266.38
 H       0.234978     5.624963    -2.056221      26.08
 H      -0.032610     5.143848     0.835383      23.89
 H      -1.261356     4.802089    -0.417745      23.05
 C      -0.901419    -0.872191    -0.161380      67.09
 H      -0.498831    -1.821245    -0.380530      21.20
 C      -2.991410     0.236768    -0.838383      44.82
 H      -4.035961     0.486947    -1.037262      20.22
 C      -2.194093     1.454527    -0.582926      -5.03
 O      -2.782123     2.744394    -0.865353      92.71
 C      -4.450159     3.004847    -0.972102      95.94
 H      -4.900419     2.718403    -0.075696      26.81
 H      -4.193224     4.135960    -0.930190      22.18
 H      -4.799322     2.257940    -1.684814      22.92
 C      -0.922817     1.553778     0.040902      31.45
 O      -0.265244     2.568629     0.396307     191.76
 C      -0.227370     0.257891     0.034797      29.82
 H       0.772147     0.204338     0.279780      19.87
 C      -2.260661    -0.956517    -0.645696       9.91
 C      -3.148682    -2.374796    -0.934887      62.26
 H      -4.194077    -2.020633    -1.515750      21.02
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 O      -2.261421    -3.182520    -1.731400     250.62
 H      -3.073594    -3.680733    -2.104588      21.69
 C      -3.763201    -3.038979     0.328434      98.78
 H      -3.039650    -3.571470     0.871418      24.68
 O      -4.664207    -1.992105     0.949266     286.58
 H      -4.738415    -2.330371     1.876999      26.07
 C      -4.786495    -4.157105    -0.052413      89.41
 O      -4.246466    -4.981592    -1.063892     282.79
 H      -3.524136    -5.601233    -0.684289      27.58
 H      -5.778188    -3.587773    -0.336364      27.54
 H      -5.015055    -4.799327     0.829636      28.14
55
name = lig-etoh-frame_852
 C       2.546679     2.013488    -2.069208      22.53
 H       1.930464     2.623663    -2.750742      20.01
 C       3.591950     1.603596     0.104834      59.14
 H       4.081696     2.059484     1.038955      23.32
 C       4.224324     0.412089    -0.435342      32.89
 O       5.042630    -0.397484     0.140149     221.71
 C       5.693430     0.081396     1.416086     103.79
 H       4.903959    -0.046216     2.254851      23.49
 H       6.052278     1.175481     1.286310      28.01
 H       6.610741    -0.576923     1.554946      25.22
 C       3.752680    -0.147911    -1.746083      15.01
 O       4.096389    -1.471249    -2.219794     139.38
 H       5.110009    -1.764967    -1.881901      23.14
 C       2.936666     0.780934    -2.500561      56.33
 H       2.671835     0.468818    -3.434948      25.28
 C       2.694911     2.423167    -0.667609      87.39
 C       2.027628     3.628082    -0.144887     109.11
 H       2.347420     4.635217    -1.000091      19.26
 O       2.132020     3.864258     1.218158     280.03
 H       3.007869     4.392159     1.351799      27.42
 C       0.599396     3.524955    -0.596614      47.10
 H       0.489747     3.224208    -1.606785      17.23
 C      -0.226341     4.936239    -0.207059      94.52
 O       0.221037     6.012413    -1.057762     256.81
 H       0.274762     5.583396    -1.958447      29.87
 H       0.130801     5.027320     0.854094      23.15
 H      -1.345464     4.934893    -0.397741      21.93
 C      -0.960025    -0.897136    -0.145357      45.21
 H      -0.375481    -1.883850    -0.236564      18.81
 C      -2.951920     0.218874    -0.861145      60.01
 H      -4.036675     0.167283    -1.023030      21.03
 C      -2.215836     1.473632    -0.572895       4.18
 O      -2.783964     2.725138    -0.872002     107.56
 C      -4.441453     2.965825    -0.907189      85.29
 H      -4.904783     2.641321     0.121333      22.56
 H      -4.253753     3.953423    -1.317238      23.72
 H      -4.552476     2.491778    -2.085276      20.26
 C      -0.941577     1.556177     0.017088      20.48
 O      -0.212562     2.597492     0.399591     167.60
 C      -0.226668     0.269658     0.015257       4.95
 H       0.786714     0.153824     0.662658      16.28
 C      -2.295228    -0.891043    -0.640870      22.23
 C      -3.152046    -2.333722    -0.961580      73.49
 H      -3.685309    -1.889401    -1.727118      22.92
 O      -2.269046    -3.200054    -1.728663     269.79
 H      -2.751833    -3.850850    -2.245066      25.96
 C      -3.872435    -3.036050     0.341846      88.69
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 H      -3.037679    -3.766023     0.843049      20.46
 O      -4.638026    -2.033646     0.955735     295.62
 H      -4.628864    -2.087422     2.081707      23.01
 C      -4.741321    -4.118363    -0.028421     103.79
 O      -4.236972    -4.989753    -1.075936     291.27
 H      -3.659213    -5.784236    -0.808435      28.01
 H      -5.688528    -3.720041    -0.218935      28.74
 H      -5.087004    -4.703696     0.904497      27.47
55
name = lig-etoh-frame_853
 C       2.483625     2.055497    -2.044360      24.35
 H       1.859815     2.602693    -2.724352      22.79
 C       3.642355     1.587952     0.127734      97.67
 H       3.898465     2.097874     0.987419      21.23
 C       4.278927     0.335440    -0.502051      12.29
 O       5.138610    -0.380335     0.183537     245.03
 C       5.658381     0.066894     1.458133     112.76
 H       5.007941    -0.055711     2.287914      27.06
 H       5.887739     1.039435     1.060896      26.76
 H       6.470264    -0.602836     1.681681      25.66
 C       3.739384    -0.159191    -1.706267      14.52
 O       4.081693    -1.485122    -2.235912     220.86
 H       4.925480    -1.702567    -1.989031      29.96
 C       2.960558     0.793832    -2.539557      73.92
 H       2.672731     0.375519    -3.599108      19.58
 C       2.661834     2.378771    -0.697488      48.57
 C       2.018043     3.705403    -0.183417     117.02
 H       2.153642     4.543405    -0.629082      25.61
 O       2.118904     3.903320     1.224521     251.67
 H       3.186193     3.935286     1.355085      27.33
 C       0.494814     3.594938    -0.636021      63.51
 H       0.347392     3.051029    -1.620783      18.30
 C      -0.208236     4.901105    -0.236705     101.74
 O       0.262601     6.017391    -1.084803     272.90
 H       0.302098     5.671558    -1.999439      30.26
 H       0.106550     5.135806     0.779428      25.92
 H      -1.292065     4.767689    -0.168423      24.56
 C      -1.002150    -0.975775    -0.175250      29.50
 H      -0.349825    -1.832353     0.141320      19.17
 C      -2.922780     0.305596    -0.867743      55.37
 H      -3.950165     0.015674    -1.129223      21.95
 C      -2.301788     1.518299    -0.574332      20.68
 O      -2.820596     2.716041    -0.867841     201.51
 C      -4.319938     2.906067    -0.907485     117.69
 H      -4.914253     2.645590    -0.095588      27.76
 H      -4.652689     3.979975    -1.368964      24.17
 H      -4.657451     2.505786    -1.855388      25.39
 C      -0.934801     1.446494    -0.058790      -7.58
 O      -0.130177     2.683108     0.414323     117.86
 C      -0.235724     0.291487     0.062376      26.56
 H       0.594315     0.273947     0.630474      17.38
 C      -2.314147    -0.972730    -0.614378      18.29
 C      -3.112213    -2.247751    -0.978817      63.76
 H      -3.733087    -1.805145    -1.897783      18.55
 O      -2.252830    -3.210748    -1.721142     221.47
 H      -2.502758    -4.150721    -2.244471      20.29
 C      -3.888420    -3.016024     0.320726      97.54
 H      -3.057875    -3.273172     0.936730      22.88
 O      -4.610948    -2.059545     1.014847     401.27
 H      -4.390903    -1.972039     1.867043      32.57
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 C      -4.768015    -4.151693    -0.001112      98.43
 O      -4.241519    -5.011232    -1.102933     306.78
 H      -3.756288    -5.734336    -0.786970      31.74
 H      -5.774516    -3.808843    -0.523432      25.15
 H      -4.945149    -4.663714     0.940656      26.89
55
name = lig-etoh-frame_854
 C       2.426624     2.039425    -2.037023      57.82
 H       1.800354     2.676588    -2.742021      22.37
 C       3.655668     1.561377     0.051113      72.26
 H       3.830545     1.905006     1.156505      19.59
 C       4.231532     0.363899    -0.530500      17.67
 O       5.263346    -0.437744     0.241199     227.22
 C       5.628128     0.062334     1.462655     108.71
 H       4.854502     0.108119     2.387023      24.99
 H       5.974006     1.151202     1.381993      27.85
 H       6.556875    -0.607046     1.807973      24.63
 C       3.720213    -0.154466    -1.724570      17.38
 O       4.024681    -1.446720    -2.255458     148.47
 H       5.039796    -1.805400    -1.820716      22.06
 C       3.000870     0.758807    -2.563550      58.85
 H       2.713013     0.454859    -3.569667      19.57
 C       2.702261     2.333611    -0.700661      29.71
 C       1.966781     3.711623    -0.241377      74.56
 H       2.466926     4.902835    -0.644785      18.45
 O       2.140285     3.937048     1.245280     301.30
 H       3.003786     3.674622     1.383247      29.40
 C       0.371041     3.633156    -0.598284      98.52
 H       0.190810     3.203155    -1.587852      19.41
 C      -0.187432     4.887625    -0.286375     104.26
 O       0.301077     6.021287    -1.101307     206.66
 H       0.266497     5.797741    -2.185410      25.48
 H       0.110440     5.262987     0.713037      24.08
 H      -1.278587     4.654497    -0.131439      23.21
 C      -0.972361    -1.029651    -0.173399      52.95
 H      -0.544388    -1.895207     0.313722      22.73
 C      -2.917346     0.340590    -0.863142      45.39
 H      -3.912672     0.330989    -1.333258      22.64
 C      -2.360113     1.536189    -0.573100      14.36
 O      -2.888676     2.758706    -0.855144     239.75
 C      -4.192168     2.884030    -0.984347     134.51
 H      -4.873554     2.559615    -0.053014      25.14
 H      -4.605893     3.884886    -0.952152      25.81
 H      -4.898790     2.021231    -1.610984      22.64
 C      -0.906107     1.431503    -0.139260     -24.91
 O      -0.085080     2.725741     0.417695      70.76
 C      -0.315558     0.236282     0.116507      40.56
 H       0.773080     0.367618     0.595170      18.03
 C      -2.305963    -1.068907    -0.588499       9.53
 C      -3.104512    -2.191746    -1.040955      84.38
 H      -3.991879    -1.957971    -1.592449      22.10
 O      -2.184593    -3.217347    -1.720152     217.08
 H      -2.713629    -4.031777    -1.764889      20.26
 C      -3.823536    -2.940062     0.265221      70.10
 H      -2.913651    -2.943217     1.001939      18.02
 O      -4.620341    -2.051035     1.067532     327.71
 H      -4.068785    -1.986569     2.017010      22.30
 C      -4.834769    -4.218981    -0.032882      90.62
 O      -4.259187    -5.037711    -1.123763     272.39
 H      -3.664819    -5.726809    -0.658891      27.44
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 H      -5.670168    -3.860684    -0.532404      27.07
 H      -4.881930    -4.783994     0.982210      25.26
55
name = lig-etoh-frame_855
 C       2.410291     1.942656    -2.065034      78.12
 H       1.868303     2.631634    -2.644878      26.48
 C       3.649793     1.538262    -0.023027      56.16
 H       3.840902     1.537293     1.008238      22.39
 C       4.189310     0.393803    -0.481887      23.56
 O       5.332969    -0.494715     0.246225     200.22
 C       5.638190     0.098218     1.531499     137.88
 H       4.778680     0.119371     2.154324      28.80
 H       6.084129     1.071422     1.754213      30.18
 H       6.432195    -0.462043     1.887380      29.47
 C       3.716953    -0.151325    -1.787968      28.46
 O       3.994470    -1.394909    -2.256023     210.92
 H       4.653846    -1.792771    -1.760996      27.62
 C       3.004984     0.758023    -2.561403      35.96
 H       2.761100     0.474195    -3.599784      18.03
 C       2.736926     2.347431    -0.705515      28.45
 C       1.956948     3.735036    -0.291061      86.46
 H       2.526161     4.374811    -0.705372      21.15
 O       2.135496     3.961219     1.248178     298.84
 H       3.108215     3.536380     1.459049      22.88
 C       0.354006     3.614290    -0.541381      98.15
 H       0.066657     3.442712    -1.608893      18.81
 C      -0.213875     4.971914    -0.310348     106.83
 O       0.325172     6.022283    -1.140084     272.24
 H       0.199615     5.822660    -2.016331      33.96
 H       0.141807     5.261780     0.696853      24.06
 H      -1.324567     4.875224    -0.370693      24.14
 C      -0.937516    -1.072074    -0.130306      47.89
 H      -0.648334    -2.114542     0.309038      19.35
 C      -2.936484     0.276664    -0.860625      44.76
 H      -3.811269     0.592039    -1.456984      21.19
 C      -2.310983     1.545068    -0.560646      -4.88
 O      -2.890908     2.813882    -0.840081     200.02
 C      -4.250581     2.811887    -1.021955     127.68
 H      -4.442963     2.481274     0.018106      25.14
 H      -4.405163     3.998419    -0.819352      22.14
 H      -4.633638     2.109139    -1.610031      26.57
 C      -0.901757     1.514881    -0.191877     -27.70
 O      -0.098540     2.689221     0.410775     145.17
 C      -0.370115     0.162389     0.178558      32.54
 H       0.665907     0.250524     0.364989      19.99
 C      -2.300852    -1.033779    -0.601550       7.56
 C      -3.124693    -2.222871    -1.078925      83.80
 H      -4.154909    -1.991648    -1.551767      20.21
 O      -2.134599    -3.200205    -1.705500     193.71
 H      -2.904828    -3.931234    -1.395075      15.94
 C      -3.732018    -2.855319     0.234872      76.43
 H      -2.863189    -3.234584     0.760876      21.53
 O      -4.635294    -2.018852     1.122977     294.71
 H      -4.127481    -2.081736     2.042132      23.74
 C      -4.818219    -4.260104    -0.068679      81.59
 O      -4.273438    -5.087646    -1.127999     282.03
 H      -3.521245    -5.652525    -0.719049      27.23
 H      -5.860486    -3.763229    -0.353602      25.22
 H      -5.020017    -4.830713     0.793183      27.55
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name = lig-etoh-frame_856
 C       2.438138     1.854059    -2.047996      91.69
 H       1.843532     2.547578    -2.731646      26.51
 C       3.633092     1.532716    -0.037836      93.04
 H       3.871397     1.602432     1.075170      19.11
 C       4.186736     0.314253    -0.494538      44.52
 O       5.348680    -0.492978     0.223636     184.11
 C       5.659164     0.132139     1.618876     104.54
 H       4.581794    -0.030209     2.082767      24.47
 H       6.107981     1.166736     1.620300      30.17
 H       6.386193    -0.687534     2.174026      25.93
 C       3.752698    -0.116843    -1.792422      37.26
 O       3.953674    -1.350356    -2.271391     101.22
 H       4.591118    -1.869420    -1.588692      20.29
 C       2.972682     0.758439    -2.585735      20.49
 H       2.809671     0.432299    -3.682730      15.93
 C       2.715095     2.381862    -0.759167      60.51
 C       1.962678     3.654835    -0.269460      88.58
 H       2.640120     4.425362    -1.061451      11.57
 O       2.129166     3.968082     1.221514     296.22
 H       3.074964     3.731121     1.436298      24.58
 C       0.416721     3.616409    -0.518271      74.88
 H       0.096410     3.422095    -1.570479      16.60
 C      -0.262460     5.099439    -0.295515     100.82
 O       0.351548     6.034746    -1.162439     244.09
 H       0.140974     5.683242    -2.182854      25.25
 H      -0.026967     5.316552     0.750410      23.44
 H      -1.332421     5.189068    -0.560969      22.78
 C      -0.972608    -1.122784    -0.066181      36.62
 H      -0.546742    -2.051501     0.109341      19.83
 C      -2.925147     0.237637    -0.853023      57.67
 H      -3.809699     0.327997    -1.502628      21.18
 C      -2.205578     1.559187    -0.561623       2.34
 O      -2.799176     2.837940    -0.838031     154.44
 C      -4.347698     2.794190    -0.943897      90.05
 H      -4.546722     2.297334     0.018133      24.25
 H      -4.549858     3.786606    -1.170981      25.85
 H      -4.593734     2.256846    -2.158617      21.26
 C      -0.896094     1.566004    -0.175409       0.82
 O      -0.163293     2.589209     0.387478     186.42
 C      -0.402831     0.153874     0.201145       8.66
 H       0.727899     0.069941     0.388835      18.39
 C      -2.326929    -0.931902    -0.664201      17.04
 C      -3.146851    -2.241195    -1.070001      83.50
 H      -3.880122    -1.945315    -1.846290      22.39
 O      -2.151168    -3.178966    -1.670079     187.86
 H      -2.613651    -4.145844    -1.470458      17.11
 C      -3.697521    -2.841286     0.242393      76.03
 H      -2.881842    -3.551032     0.653271      20.18
 O      -4.614976    -1.997747     1.146922     272.35
 H      -4.394683    -2.120275     2.139711      24.04
 C      -4.773633    -4.226266    -0.111645      90.72
 O      -4.281710    -5.143775    -1.131687     293.53
 H      -3.496663    -5.591100    -0.900554      30.66
 H      -5.742369    -3.800882    -0.255382      27.40
 H      -5.064067    -4.897054     0.825013      26.49
55
name = lig-etoh-frame_857
 C       2.433747     1.869664    -2.043935      73.33
 H       1.821127     2.334110    -2.776953      22.23
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 C       3.613836     1.532554     0.003749     168.85
 H       3.827468     2.019897     0.972039      21.20
 C       4.216055     0.224164    -0.512989      34.63
 O       5.328626    -0.443527     0.197853     202.59
 C       5.650127     0.101180     1.690069     109.64
 H       4.739001     0.096761     2.169469      29.20
 H       5.982759     1.086692     1.398584      28.14
 H       6.159280    -0.603511     2.178145      28.47
 C       3.795266    -0.073884    -1.772056      27.21
 O       3.931920    -1.343767    -2.291100     155.47
 H       4.577342    -1.898813    -1.616353      16.14
 C       2.962992     0.698189    -2.633499     -43.00
 H       2.786272     0.432050    -3.610573      20.87
 C       2.696120     2.355089    -0.789240      86.68
 C       2.010251     3.576032    -0.245652     135.39
 H       2.123356     4.458186    -0.768545      18.84
 O       2.124526     3.967151     1.158383     311.62
 H       3.080139     4.036642     1.356979      29.94
 C       0.462251     3.654904    -0.506603      40.00
 H       0.301923     3.240187    -1.499492      17.50
 C      -0.298711     5.191286    -0.269618      87.88
 O       0.388422     6.062286    -1.200324     272.03
 H       0.314257     5.603327    -2.101002      28.27
 H      -0.290249     5.549468     0.802627      23.25
 H      -1.386683     5.201943    -0.559228      22.47
 C      -1.074701    -1.081481    -0.021546      31.53
 H      -0.356668    -2.033051    -0.096211      16.61
 C      -2.900000     0.316582    -0.865742      54.41
 H      -3.838517     0.039815    -1.377402      19.49
 C      -2.163358     1.567860    -0.606965      10.22
 O      -2.718933     2.838821    -0.839049     121.77
 C      -4.376637     2.754907    -0.925821      94.71
 H      -5.063537     2.149033    -0.229365      24.17
 H      -4.897822     3.774987    -1.332586      23.60
 H      -4.558626     2.466659    -1.853158      25.95
 C      -0.866924     1.496614    -0.097227      26.99
 O      -0.221898     2.510200     0.361869     168.22
 C      -0.386369     0.158170     0.188964      11.45
 H       0.647098     0.033832     0.607681      17.62
 C      -2.324722    -0.938389    -0.716684      17.61
 C      -3.130740    -2.214324    -1.045532      77.59
 H      -3.673760    -1.983916    -2.006166      20.57
 O      -2.180777    -3.175724    -1.627742     273.57
 H      -2.305102    -4.089537    -1.726020      24.75
 C      -3.749388    -2.921334     0.270743      74.85
 H      -2.906536    -3.392927     0.787218      23.62
 O      -4.549380    -1.989445     1.133775     277.31
 H      -4.678240    -2.266879     2.192704      24.05
 C      -4.702446    -4.180402    -0.108797      95.71
 O      -4.306917    -5.186952    -1.149729     276.97
 H      -3.391609    -5.661621    -0.942779      26.45
 H      -5.697489    -3.777715    -0.550140      25.99
 H      -4.789629    -4.690590     0.799308      28.80
55
name = lig-etoh-frame_858
 C       2.411967     1.884256    -2.122061      53.75
 H       1.659036     2.388002    -2.785936      18.75
 C       3.599989     1.528189     0.030206      83.42
 H       3.877365     2.172544     0.862314      21.86
 C       4.248602     0.256461    -0.434073      32.92
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 O       5.282685    -0.390337     0.185110     208.64
 C       5.583080     0.069029     1.669155      89.49
 H       4.660520     0.388258     2.389791      24.08
 H       6.072117     1.067956     1.448574      25.65
 H       6.385019    -0.720381     2.180918      24.15
 C       3.814660    -0.091452    -1.805399      39.66
 O       3.936959    -1.371568    -2.305802     157.38
 H       4.593043    -1.843203    -1.879167      20.03
 C       2.971927     0.670188    -2.609510      48.98
 H       2.668762     0.308681    -3.711613      24.47
 C       2.713765     2.275296    -0.766987      61.05
 C       1.993294     3.543085    -0.201503     113.74
 H       2.064558     4.700006    -0.768669      16.11
 O       2.142428     3.944997     1.103188     243.74
 H       3.084418     4.498487     1.250948      26.00
 C       0.459886     3.666642    -0.472592      23.32
 H       0.425037     3.256340    -1.536201      15.42
 C      -0.319305     5.226966    -0.266078      87.54
 O       0.432318     6.099891    -1.211685     235.07
 H       0.501564     5.608161    -2.146295      26.71
 H      -0.327336     5.744795     0.685304      23.75
 H      -1.357261     4.972169    -0.516323      23.29
 C      -1.140590    -1.003557    -0.020948      58.84
 H      -0.552509    -1.827660    -0.122841      20.24
 C      -2.871364     0.403953    -0.905741      49.86
 H      -3.948326     0.297732    -1.175424      21.01
 C      -2.191603     1.544138    -0.679248       9.97
 O      -2.706547     2.833895    -0.828975      95.41
 C      -4.387078     2.761256    -0.935833      76.76
 H      -5.155533     2.188607    -0.441300      24.94
 H      -4.807603     3.715716    -0.859509      25.38
 H      -4.472680     2.064466    -2.076500      19.86
 C      -0.867792     1.338648    -0.024643      10.07
 O      -0.230922     2.512810     0.370003     132.09
 C      -0.351869     0.136209     0.186499      54.40
 H       0.560012     0.138135     0.765970      18.34
 C      -2.295513    -0.994196    -0.722255      25.16
 C      -3.104554    -2.201642    -1.023756      71.68
 H      -3.881885    -2.012627    -1.833076      21.00
 O      -2.164493    -3.150183    -1.584540     184.66
 H      -2.387653    -4.214437    -2.009966      18.13
 C      -3.828874    -2.999674     0.285382      66.11
 H      -2.876127    -3.120226     0.952370      20.21
 O      -4.482079    -1.997230     1.102907     343.69
 H      -4.572357    -2.388526     1.901396      30.28
 C      -4.634198    -4.124795    -0.122330      94.31
 O      -4.317107    -5.222681    -1.161459     265.98
 H      -3.467490    -5.679499    -0.923010      28.23
 H      -5.515060    -3.815184    -0.697999      25.63
 H      -4.717035    -4.595386     0.951014      25.06
55
name = lig-etoh-frame_859
 C       2.393122     1.881373    -2.196275       5.80
 H       1.632755     2.494035    -2.681830      15.75
 C       3.613345     1.510051     0.041212      37.40
 H       4.044927     2.040055     0.958306      21.43
 C       4.224651     0.379379    -0.382306      44.91
 O       5.231959    -0.350390     0.220926     229.57
 C       5.527257     0.056301     1.622523     142.06
 H       4.790436     0.345664     2.260624      28.34
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 H       6.205456     0.917747     1.648799      29.28
 H       6.224009    -0.594680     1.909617      29.77
 C       3.831072    -0.141062    -1.805580      34.77
 O       3.946330    -1.414863    -2.329867     113.66
 H       4.951060    -1.899848    -2.031203      19.00
 C       2.959531     0.682851    -2.594536      36.14
 H       2.675633     0.220908    -3.449829      26.92
 C       2.700286     2.212776    -0.774488      47.30
 C       1.933153     3.605674    -0.214092     119.07
 H       2.421282     4.255890    -0.864042      23.75
 O       2.200326     3.934188     1.110838     323.87
 H       2.864148     4.555493     1.118239      31.60
 C       0.432502     3.633130    -0.435221      56.26
 H       0.247648     3.534409    -1.492498      18.37
 C      -0.292477     5.199627    -0.309280      85.85
 O       0.459670     6.132420    -1.199302     220.50
 H       0.610433     5.702539    -2.168035      27.14
 H      -0.190318     5.786167     0.647620      23.23
 H      -1.323312     4.831009    -0.598262      22.45
 C      -1.139219    -0.962492    -0.048883      47.99
 H      -0.679298    -2.060820     0.090092      18.48
 C      -2.890565     0.376618    -0.965517      50.76
 H      -3.923224     0.714080    -1.044288      20.46
 C      -2.187268     1.522013    -0.719639       1.36
 O      -2.759864     2.816421    -0.800434     135.50
 C      -4.360221     2.738672    -1.032580      94.12
 H      -4.815028     2.050856    -0.178341      23.52
 H      -4.476232     3.855917    -0.572247      21.37
 H      -4.411055     2.312606    -1.887988      24.99
 C      -0.914666     1.309513    -0.011198      -7.69
 O      -0.222578     2.543286     0.406104     130.57
 C      -0.303943     0.093030     0.222928      45.78
 H       0.646531     0.138206     0.903942      17.29
 C      -2.329145    -0.960351    -0.715431      33.33
 C      -3.123468    -2.239398    -0.999900      80.24
 H      -4.079887    -1.975340    -1.529875      21.93
 O      -2.108293    -3.159054    -1.573788     269.76
 H      -2.784644    -3.718249    -1.896553      23.27
 C      -3.779294    -2.966740     0.268855      85.34
 H      -2.908155    -3.219051     0.892090      22.71
 O      -4.441666    -2.005325     1.041485     308.38
 H      -4.463926    -2.477595     2.016248      24.15
 C      -4.609269    -4.152318    -0.130858     108.36
 O      -4.307084    -5.238938    -1.150882     334.74
 H      -3.511622    -5.725339    -0.898543      30.64
 H      -5.552730    -3.706785    -0.534044      27.26
 H      -5.007803    -4.629966     0.745906      28.26
55
name = lig-etoh-frame_860
 C       2.390904     1.891389    -2.161554      23.78
 H       1.690887     2.497245    -2.735413      16.58
 C       3.622777     1.548832     0.069830      54.71
 H       3.983572     1.831980     1.006413      20.63
 C       4.197005     0.426165    -0.451433      35.86
 O       5.173172    -0.307845     0.283961     223.25
 C       5.520074     0.070630     1.534841     109.13
 H       4.544490     0.154816     2.265407      22.67
 H       6.242052     0.926756     1.674188      27.09
 H       6.134662    -0.963609     1.918553      23.53
 C       3.823914    -0.145284    -1.752099      43.78
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 O       4.004334    -1.480920    -2.340060     218.32
 H       4.869043    -1.724609    -2.161301      27.66
 C       2.965412     0.667825    -2.573118      64.11
 H       2.612721     0.073212    -3.534819      22.56
 C       2.629566     2.200670    -0.813141      43.13
 C       1.906970     3.621061    -0.263254     117.48
 H       2.648519     4.096629    -0.995028      24.35
 O       2.246288     3.918519     1.149385     290.38
 H       2.987727     4.608627     1.132860      29.74
 C       0.378543     3.615517    -0.412239      85.46
 H      -0.025391     3.578107    -1.476035      17.33
 C      -0.221736     5.131838    -0.358672     100.43
 O       0.476667     6.150759    -1.175338     270.24
 H       0.502162     5.805545    -2.085974      31.62
 H      -0.168725     5.541491     0.636775      25.59
 H      -1.257617     5.043712    -0.688095      24.57
 C      -1.074621    -1.039541    -0.083558      20.07
 H      -0.956007    -1.979432     0.393935      19.97
 C      -2.935808     0.312338    -1.023808      57.15
 H      -3.991000     0.621433    -1.151261      20.73
 C      -2.139069     1.512846    -0.714076       6.54
 O      -2.830153     2.771531    -0.772422     159.07
 C      -4.263328     2.750150    -1.009987      97.32
 H      -4.371087     2.069862    -0.240520      24.30
 H      -4.389310     3.766121    -0.821559      25.18
 H      -4.653176     2.633055    -2.335839      20.91
 C      -0.938273     1.412943    -0.042364      -4.22
 O      -0.215385     2.574462     0.454578     153.37
 C      -0.265956     0.089033     0.291751      25.31
 H       0.621965    -0.020537     0.791500      21.23
 C      -2.428107    -0.876926    -0.709244       9.06
 C      -3.135687    -2.252474    -0.941135      85.63
 H      -4.078192    -1.982409    -1.546849      19.88
 O      -2.088082    -3.161494    -1.582342     234.60
 H      -2.965550    -3.663461    -1.943387      18.28
 C      -3.625494    -2.920305     0.241018      91.19
 H      -2.777748    -3.519251     0.805549      19.81
 O      -4.434416    -2.022887     1.002606     310.11
 H      -4.389080    -2.156213     2.026322      25.24
 C      -4.662568    -4.220869    -0.152498      85.04
 O      -4.288517    -5.224166    -1.128683     297.81
 H      -3.438992    -5.801093    -0.842294      25.31
 H      -5.565358    -3.573530    -0.441980      26.29
 H      -5.203539    -4.792041     0.685604      26.46
55
name = lig-etoh-frame_861
 C       2.399561     1.874522    -2.094161      50.99
 H       1.789963     2.408916    -2.868410      19.97
 C       3.579498     1.617132     0.040948      94.59
 H       3.751928     1.861007     1.173145      16.82
 C       4.204522     0.396424    -0.541668      18.12
 O       5.098598    -0.276943     0.280630     247.56
 C       5.530928     0.038482     1.545859     135.32
 H       4.658549     0.047050     2.100375      28.83
 H       6.105892     0.945736     1.584332      28.69
 H       5.828703    -0.844811     1.915142      27.99
 C       3.781000    -0.136708    -1.728060      21.38
 O       4.057413    -1.508145    -2.327636     177.67
 H       5.058452    -1.752212    -2.103737      25.04
 C       2.972063     0.607501    -2.567012      50.99
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 H       2.650828     0.223583    -3.496189      23.56
 C       2.554676     2.241360    -0.779966      64.57
 C       1.935926     3.566387    -0.307047     101.24
 H       2.409253     4.441783    -0.929067      23.03
 O       2.273452     3.905229     1.164932     214.64
 H       3.222781     4.433794     1.259922      27.48
 C       0.316207     3.638276    -0.454271      70.52
 H       0.004474     3.160284    -1.394857      20.41
 C      -0.156321     5.068744    -0.375288     105.66
 O       0.498296     6.151717    -1.124748     223.76
 H       0.320031     5.872799    -2.197251      23.99
 H      -0.194418     5.301429     0.730902      25.24
 H      -1.216374     5.280102    -0.723890      23.01
 C      -1.041296    -1.079322    -0.102591      19.03
 H      -0.983880    -2.015437     0.548682      19.52
 C      -2.977476     0.334031    -1.070827      57.89
 H      -3.999428     0.179977    -1.480266      21.76
 C      -2.150322     1.500670    -0.702069       8.04
 O      -2.841431     2.722030    -0.766335     199.46
 C      -4.148105     2.778367    -1.043316     120.21
 H      -4.706844     1.952002    -0.310612      24.32
 H      -4.626638     3.898702    -0.904349      23.94
 H      -4.624008     2.751228    -1.913126      27.46
 C      -0.869077     1.512807    -0.057822      -0.16
 O      -0.218593     2.610677     0.508973     150.21
 C      -0.330470     0.109174     0.310237       3.41
 H       0.769432    -0.102839     0.745905      19.88
 C      -2.461300    -0.884333    -0.671005      -5.84
 C      -3.110552    -2.199393    -0.917949      85.05
 H      -3.882490    -2.119116    -1.701029      20.77
 O      -2.132133    -3.153464    -1.608776     184.68
 H      -2.567449    -4.023516    -2.144007      19.32
 C      -3.507003    -2.971294     0.284773      83.24
 H      -2.691400    -3.564289     0.748652      21.75
 O      -4.426603    -2.030716     0.979662     331.66
 H      -4.292030    -1.982947     1.916494      29.26
 C      -4.743732    -4.262943    -0.153631      85.44
 O      -4.259151    -5.201822    -1.114498     329.43
 H      -3.500137    -5.678459    -0.816800      29.73
 H      -5.486295    -3.664445    -0.656768      27.58
 H      -5.014544    -4.773770     0.772580      26.89
55
name = lig-etoh-frame_862
 C       2.409875     1.799367    -2.080805      46.98
 H       1.882656     2.338389    -2.832308      22.66
 C       3.516552     1.640358    -0.023640      66.90
 H       3.503214     1.929359     0.968861      18.91
 C       4.199585     0.423289    -0.525351      27.52
 O       5.035464    -0.291706     0.201695     225.99
 C       5.500156     0.020681     1.583945      92.53
 H       4.543369     0.293881     2.282729      24.53
 H       6.104337     0.989989     1.598653      26.49
 H       6.079341    -0.965659     2.029474      24.00
 C       3.746277    -0.200213    -1.772151      28.06
 O       4.119820    -1.492596    -2.288639     146.31
 H       5.093302    -1.816505    -1.894210      23.60
 C       2.943832     0.605536    -2.546242      57.05
 H       2.703191     0.312058    -3.609335      22.93
 C       2.526485     2.310612    -0.701939      61.85
 C       1.955918     3.551766    -0.308311     101.52
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 H       2.044824     4.592229    -0.789819      19.69
 O       2.295140     3.888011     1.155643     289.59
 H       3.201999     4.014780     1.263514      31.41
 C       0.314326     3.616659    -0.540571      51.53
 H       0.215230     2.914362    -1.386960      20.73
 C      -0.158449     5.052204    -0.355462     107.92
 O       0.529735     6.134305    -1.082849     274.48
 H       0.379226     5.959089    -1.963347      32.55
 H      -0.090301     5.217642     0.711424      25.60
 H      -1.190130     5.132941    -0.631351      24.75
 C      -1.083455    -1.047412    -0.083513      50.34
 H      -0.731337    -2.002197     0.406432      21.08
 C      -2.977043     0.347515    -1.090573      51.71
 H      -3.783020     0.099693    -1.814044      22.14
 C      -2.219181     1.494400    -0.690296      -5.31
 O      -2.779395     2.699574    -0.768440     179.97
 C      -4.147316     2.823950    -1.003033     115.38
 H      -4.979086     2.269754    -0.656663      26.14
 H      -4.559271     3.728156    -0.666686      26.83
 H      -4.515069     2.449048    -2.279774      22.53
 C      -0.788043     1.514845    -0.053035     -23.15
 O      -0.236541     2.659951     0.566982     145.26
 C      -0.406507     0.143597     0.283889      35.43
 H       0.539520     0.083028     0.657347      23.05
 C      -2.384646    -0.937320    -0.620410       4.80
 C      -3.073650    -2.195959    -0.954384      74.56
 H      -3.906396    -2.178596    -1.756695      20.12
 O      -2.150713    -3.156265    -1.662926     276.95
 H      -2.366580    -3.925216    -1.984765      26.68
 C      -3.518676    -3.056805     0.334404      63.65
 H      -2.570911    -3.444205     0.915607      20.95
 O      -4.404716    -2.047652     0.961013     309.83
 H      -4.134624    -1.907522     2.027324      24.26
 C      -4.750344    -4.263835    -0.142315      75.76
 O      -4.239708    -5.181021    -1.113744     308.38
 H      -3.419733    -5.666728    -0.759294      26.10
 H      -5.565780    -3.769106    -0.816554      24.63
 H      -4.913280    -4.639566     0.890623      25.25
55
name = lig-etoh-frame_863
 C       2.390838     1.758371    -2.057207      47.89
 H       1.843318     2.396016    -2.809086      22.88
 C       3.472633     1.607264    -0.071943      57.72
 H       3.589548     1.952237     1.028478      19.50
 C       4.116868     0.479066    -0.511793      31.78
 O       5.023050    -0.349497     0.160861     217.77
 C       5.435185     0.010817     1.631703     128.12
 H       4.730394     0.385457     2.286340      28.12
 H       6.125719     0.829285     1.574131      28.80
 H       6.157753    -0.676093     1.894736      28.28
 C       3.750804    -0.270941    -1.790166      15.22
 O       4.191860    -1.458646    -2.229045     217.66
 H       4.876312    -1.776757    -1.715296      27.76
 C       2.896389     0.603925    -2.556958      66.39
 H       2.795877     0.394591    -3.656745      23.68
 C       2.543219     2.334386    -0.748067      29.79
 C       1.918497     3.617284    -0.244448      97.69
 H       2.095382     4.581015    -0.907381      16.35
 O       2.282691     3.861275     1.127466     307.65
 H       3.343665     3.671893     1.196284      23.24
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 C       0.390226     3.535579    -0.580196      60.40
 H       0.278343     3.079168    -1.601884      19.51
 C      -0.195122     5.045536    -0.337142      88.09
 O       0.565362     6.109352    -1.005401     201.45
 H       0.509588     5.914586    -2.108841      23.54
 H       0.063852     5.266822     0.731949      22.95
 H      -1.319862     4.918425    -0.517784      22.42
 C      -1.132290    -0.986750    -0.026873      79.68
 H      -0.538768    -1.898726     0.104736      22.60
 C      -2.899267     0.289392    -1.073575      71.80
 H      -3.595508     0.424184    -1.920882      25.23
 C      -2.250953     1.466777    -0.661898     -22.70
 O      -2.724877     2.722099    -0.763041     129.52
 C      -4.209877     2.853837    -1.048782      93.56
 H      -5.004009     2.111884    -0.567364      23.50
 H      -4.344163     3.974350    -0.603487      22.95
 H      -4.133016     2.586720    -2.142478      23.05
 C      -0.810080     1.447332    -0.042782     -45.12
 O      -0.270285     2.703081     0.595022     122.46
 C      -0.460023     0.223748     0.233897      66.24
 H       0.578393     0.192694     0.790810      22.18
 C      -2.307257    -0.966846    -0.621983      19.73
 C      -3.055655    -2.302305    -1.006219      74.51
 H      -3.985586    -2.006989    -1.520674      22.43
 O      -2.108692    -3.117101    -1.724398     157.52
 H      -2.703825    -4.151264    -1.810688      13.42
 C      -3.616196    -3.110101     0.328249      85.99
 H      -2.746845    -3.233149     1.026885      21.88
 O      -4.366740    -2.069802     0.984107     378.71
 H      -4.150777    -1.992468     1.885415      30.06
 C      -4.679491    -4.219209    -0.127456      99.11
 O      -4.217168    -5.176613    -1.109846     326.29
 H      -3.385639    -5.727387    -0.794169      26.57
 H      -5.567336    -3.794328    -0.496921      27.55
 H      -5.091143    -4.613546     0.848234      26.12
55
name = lig-etoh-frame_864
 C       2.319481     1.800183    -2.052689      71.74
 H       1.776325     2.379685    -2.764429      24.27
 C       3.451480     1.579265    -0.025278      91.91
 H       3.887894     1.811401     0.924894      25.06
 C       4.028468     0.427588    -0.549205      21.53
 O       5.026079    -0.404213     0.183994     194.59
 C       5.402901     0.031733     1.600558      95.70
 H       4.570808     0.290906     2.421170      23.55
 H       6.126722     0.897792     1.417135      26.07
 H       6.130196    -0.848993     1.941239      24.56
 C       3.731195    -0.224307    -1.761730      18.30
 O       4.254042    -1.424739    -2.184380     168.03
 H       4.863318    -1.875379    -1.324410      19.26
 C       2.888243     0.543906    -2.591301      55.46
 H       2.763285     0.402535    -3.638612      22.72
 C       2.573048     2.338957    -0.866093      46.96
 C       1.881011     3.670015    -0.212145     122.79
 H       2.381296     4.464461    -0.930403      16.78
 O       2.264228     3.831649     1.097885     374.97
 H       3.242289     3.625889     1.140622      26.41
 C       0.466538     3.497946    -0.541204      82.58
 H       0.223664     3.330183    -1.590205      19.68
 C      -0.218661     5.006311    -0.310876      97.43
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 O       0.578325     6.071817    -0.958327     248.93
 H       0.709613     5.846110    -1.888981      30.10
 H       0.020170     5.254585     0.717582      24.38
 H      -1.284073     4.955987    -0.440409      25.06
 C      -1.111003    -0.936062     0.057769      43.31
 H      -0.418741    -1.856101    -0.160532      19.85
 C      -2.793991     0.235511    -1.045864      65.80
 H      -3.578328     0.568005    -1.743618      24.16
 C      -2.203376     1.443720    -0.609196       6.20
 O      -2.705099     2.757029    -0.747374     135.54
 C      -4.260248     2.891656    -1.068854     104.34
 H      -4.614925     2.115484    -0.501239      24.16
 H      -4.248319     3.962331    -0.911146      24.57
 H      -3.997218     3.000471    -2.306494      20.72
 C      -0.962530     1.475348    -0.032216       6.90
 O      -0.312892     2.707138     0.552564     132.87
 C      -0.398562     0.253077     0.241730      26.53
 H       0.468285     0.168524     0.839947      21.70
 C      -2.328806    -1.014196    -0.695401       3.10
 C      -3.035128    -2.398760    -1.013523      81.35
 H      -4.001160    -1.893477    -1.406622      21.92
 O      -2.090707    -3.128396    -1.803858     268.83
 H      -2.688050    -3.809450    -1.677293      23.18
 C      -3.715024    -3.099305     0.282999     104.26
 H      -2.901983    -3.451003     0.982476      22.69
 O      -4.353340    -2.085132     1.005548     339.93
 H      -4.158643    -2.141811     1.990678      27.02
 C      -4.589976    -4.180289    -0.065347     103.87
 O      -4.187732    -5.175479    -1.105602     334.03
 H      -3.486813    -5.749929    -0.845527      30.69
 H      -5.577458    -3.589988    -0.360891      25.36
 H      -5.098014    -4.785275     0.717535      26.48
55
name = lig-etoh-frame_865
 C       2.249280     1.803701    -2.146630      89.73
 H       1.578048     2.368413    -2.841444      23.70
 C       3.451814     1.541155     0.013254     108.27
 H       4.020856     1.857837     0.915851      24.82
 C       3.986465     0.314350    -0.529652       9.78
 O       5.004562    -0.439980     0.235261     207.58
 C       5.408245     0.044508     1.537772     122.11
 H       4.557289     0.058363     2.183076      26.46
 H       5.933217     0.962356     1.441196      28.02
 H       5.787848    -0.861108     1.983656      25.86
 C       3.689665    -0.153773    -1.762886      19.47
 O       4.317202    -1.394146    -2.119285     231.23
 H       4.725784    -1.789959    -1.371289      24.05
 C       2.870846     0.527929    -2.607474      32.94
 H       2.636010     0.222497    -3.717587      20.52
 C       2.621989     2.352965    -0.879941      48.64
 C       1.921782     3.643756    -0.265846     128.80
 H       2.532050     4.456083    -0.832894      17.52
 O       2.230527     3.804391     1.094113     411.51
 H       3.167842     3.827319     1.189959      29.20
 C       0.445685     3.563898    -0.446580      78.63
 H       0.190671     3.298501    -1.515721      19.95
 C      -0.189253     4.954945    -0.263448     100.65
 O       0.574660     6.029607    -0.906717     251.63
 H       0.763634     5.744793    -1.884643      27.62
 H      -0.178496     5.176093     0.839974      24.62
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 H      -1.288607     5.071568    -0.555577      24.29
 C      -1.054944    -0.940113     0.082083      27.05
 H      -0.477901    -1.802238     0.016379      21.28
 C      -2.735457     0.231257    -1.037621      62.63
 H      -3.745022     0.313023    -1.504190      24.65
 C      -2.182396     1.475389    -0.578811      28.71
 O      -2.712885     2.780139    -0.734159     166.40
 C      -4.184386     2.963236    -1.145846      99.60
 H      -4.652396     2.060569    -0.481038      22.94
 H      -4.531693     4.038815    -0.883217      24.77
 H      -4.388900     2.974687    -2.248516      25.14
 C      -1.046305     1.553489     0.043150      21.97
 O      -0.357474     2.677976     0.454882     177.88
 C      -0.327044     0.250307     0.286956      -6.61
 H       0.644555     0.190618     0.855737      20.03
 C      -2.337241    -1.073804    -0.736194       7.27
 C      -3.028249    -2.370729    -0.982807      87.88
 H      -3.882791    -2.158213    -1.672544      22.68
 O      -2.096601    -3.148475    -1.878613     161.33
 H      -2.600131    -4.200418    -1.937381      15.22
 C      -3.684943    -3.063106     0.267339      97.94
 H      -2.926111    -3.777856     0.782577      21.00
 O      -4.365618    -2.076286     1.038451     302.98
 H      -4.228285    -2.381166     2.080699      24.73
 C      -4.612117    -4.194031    -0.028274      99.85
 O      -4.168695    -5.141149    -1.111277     292.58
 H      -3.431105    -5.842216    -0.764718      25.84
 H      -5.371721    -3.654569    -0.505392      27.59
 H      -4.835040    -4.911322     0.807335      27.17
55
name = lig-etoh-frame_866
 C       2.218899     1.775744    -2.252484      55.89
 H       1.448544     2.256063    -2.860811      21.54
 C       3.474069     1.487575     0.000990      76.21
 H       3.846675     2.055392     0.901117      21.81
 C       3.977552     0.250747    -0.401098      26.20
 O       4.956698    -0.471692     0.256512     228.80
 C       5.378222     0.024096     1.471452     111.41
 H       4.352225     0.157745     2.045292      24.26
 H       5.904426     1.044656     1.606564      25.32
 H       5.922724    -0.826600     2.003145      25.83
 C       3.681398    -0.167384    -1.786630      15.40
 O       4.340239    -1.337041    -2.085136     168.15
 H       4.812025    -1.719140    -1.281413      20.86
 C       2.795432     0.579314    -2.657108      49.09
 H       2.579141     0.039915    -3.510028      24.03
 C       2.657860     2.327725    -0.852954      55.99
 C       2.028500     3.564838    -0.331571     103.24
 H       2.348619     4.583623    -0.830863      17.75
 O       2.189485     3.771586     1.114500     281.98
 H       3.176989     4.264143     1.347079      24.43
 C       0.356043     3.649656    -0.401437      64.13
 H       0.221784     3.199897    -1.361336      21.53
 C      -0.175303     4.948881    -0.189384     118.59
 O       0.573978     5.984261    -0.852846     252.20
 H       0.614242     5.688803    -1.894014      25.09
 H      -0.354171     5.134368     0.872049      25.65
 H      -1.118956     4.983775    -0.732851      24.38
 C      -1.000450    -0.974668     0.040573      32.37
 H      -0.465344    -1.988951     0.493270      20.60
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 C      -2.763607     0.234555    -1.041558      57.28
 H      -3.811154     0.077707    -1.309294      24.90
 C      -2.259882     1.528906    -0.604802      -8.38
 O      -2.759764     2.815034    -0.750839     209.54
 C      -4.076842     3.026082    -1.193024     148.08
 H      -4.813544     2.391368    -0.768259      26.34
 H      -4.708345     3.788319    -0.653765      25.49
 H      -4.758584     2.616307    -2.151094      22.73
 C      -0.950614     1.544005     0.170363      15.19
 O      -0.382669     2.670646     0.376172     189.36
 C      -0.315015     0.262883     0.348615      28.21
 H       0.772625     0.303016     0.671924      21.37
 C      -2.254965    -1.063538    -0.699271      14.51
 C      -3.045920    -2.329023    -1.001027      76.20
 H      -3.764563    -2.381299    -1.844493      18.40
 O      -2.126310    -3.208445    -1.928916     231.88
 H      -2.254336    -4.140872    -2.292366      24.46
 C      -3.575256    -3.064625     0.270849      82.61
 H      -2.712669    -3.571213     0.741723      22.91
 O      -4.370392    -2.078669     1.098528     323.99
 H      -4.399162    -2.362056     1.948594      30.85
 C      -4.664073    -4.247664    -0.048597      91.32
 O      -4.135071    -5.106661    -1.114125     336.63
 H      -3.485057    -5.725022    -0.756455      29.16
 H      -5.619238    -3.885038    -0.635046      25.18
 H      -4.738813    -4.699201     0.939373      27.41
55
name = lig-etoh-frame_867
 C       2.221818     1.777546    -2.267204      44.77
 H       1.414437     2.195590    -2.868033      21.18
 C       3.485479     1.490313    -0.021342      62.34
 H       3.598472     2.035073     0.878792      22.29
 C       3.951373     0.224917    -0.337674      31.39
 O       4.914607    -0.517452     0.239331     259.29
 C       5.312861     0.001162     1.495119     122.67
 H       4.443201     0.315074     2.045895      27.67
 H       5.884971     0.924077     1.484728      27.69
 H       6.133619    -0.614542     1.944872      26.85
 C       3.686563    -0.176835    -1.739990      12.69
 O       4.338729    -1.291198    -2.090152     132.02
 H       5.025838    -1.543420    -1.234148      18.51
 C       2.749723     0.585350    -2.680797      68.25
 H       2.418809    -0.099823    -3.572947      24.10
 C       2.661502     2.236213    -0.894156      63.83
 C       2.101572     3.518801    -0.341729     107.60
 H       2.049676     4.538727    -0.867878      19.02
 O       2.187586     3.753378     1.145524     326.44
 H       2.797817     4.397172     1.368657      32.00
 C       0.336731     3.620924    -0.427549      51.04
 H       0.144221     3.319486    -1.528732      20.80
 C      -0.217620     5.004703    -0.132409     111.63
 O       0.585843     5.949819    -0.811284     282.51
 H       0.457383     5.779456    -1.720375      31.16
 H      -0.414118     5.234619     0.925627      25.48
 H      -1.175741     4.850342    -0.717221      23.61
 C      -0.927101    -1.047997     0.014089      70.99
 H      -0.661434    -1.782688     0.636983      24.86
 C      -2.834937     0.254441    -1.023220      53.62
 H      -3.885898     0.120654    -1.328352      24.07
 C      -2.299793     1.530594    -0.607181     -24.95
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 O      -2.808221     2.848616    -0.787644     169.82
 C      -4.094533     3.042117    -1.222644     124.72
 H      -4.843180     2.279794    -0.626825      24.34
 H      -4.454709     3.926017    -0.685921      24.76
 H      -4.329491     2.678063    -2.233093      24.96
 C      -0.905087     1.440293     0.193668       0.97
 O      -0.372755     2.724161     0.380261     170.04
 C      -0.327087     0.268396     0.401619      52.90
 H       0.717311     0.312051     0.570037      23.82
 C      -2.124384    -1.002666    -0.636275      -4.01
 C      -3.056308    -2.335731    -1.059670      56.80
 H      -3.926717    -2.093225    -1.712579      21.20
 O      -2.105792    -3.247927    -1.971845     230.24
 H      -2.415179    -4.068521    -2.311655      24.12
 C      -3.519422    -3.077129     0.265470      69.73
 H      -2.505809    -3.201626     0.851394      20.31
 O      -4.350401    -2.086934     1.127354     265.24
 H      -4.529013    -2.383456     2.141540      25.55
 C      -4.680188    -4.271925    -0.111319      92.49
 O      -4.112982    -5.082763    -1.107764     350.42
 H      -3.383562    -5.686381    -0.781977      27.76
 H      -5.705446    -4.049465    -0.316962      27.37
 H      -4.898566    -4.566853     0.980493      26.56
55
name = lig-etoh-frame_868
 C       2.241796     1.787473    -2.217986      38.02
 H       1.457224     2.299042    -2.825393      20.17
 C       3.472389     1.524862    -0.040691      79.01
 H       3.475406     1.926787     1.046986      19.04
 C       3.895114     0.229405    -0.390660      21.91
 O       4.888885    -0.581787     0.235939     218.10
 C       5.290984     0.004839     1.546900      96.76
 H       4.470416     0.255857     2.314370      27.15
 H       5.834999     0.950648     1.126836      25.21
 H       6.043347    -0.648666     1.969549      27.71
 C       3.655443    -0.142804    -1.674179      23.44
 O       4.351084    -1.275294    -2.107836     220.80
 H       5.012175    -1.386932    -1.548328      27.88
 C       2.760083     0.491010    -2.664508      48.57
 H       2.356937     0.116830    -3.560685      26.31
 C       2.631475     2.159741    -0.973627      56.33
 C       2.057734     3.507959    -0.305507     113.99
 H       2.266156     4.409065    -0.936161      23.90
 O       2.183280     3.718120     1.155648     289.70
 H       2.746683     4.539289     1.348423      28.71
 C       0.378832     3.530021    -0.507476      61.53
 H       0.055385     3.569671    -1.542229      21.27
 C      -0.290854     5.039253    -0.109591      93.55
 O       0.605363     5.948302    -0.763110     213.65
 H       0.330129     5.919298    -1.837070      26.10
 H      -0.341583     5.354704     0.958947      25.65
 H      -1.345826     4.959964    -0.450650      25.02
 C      -0.853577    -1.052658     0.017186      51.15
 H      -0.632430    -2.025395     0.721642      21.06
 C      -2.883982     0.291963    -0.965376      56.12
 H      -3.854366     0.266641    -1.474596      23.05
 C      -2.293340     1.493054    -0.580554      -5.34
 O      -2.796172     2.844581    -0.806824     149.28
 C      -4.213939     3.003249    -1.214177     107.54
 H      -4.641850     2.291372    -0.631244      24.56
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 H      -4.190185     4.185379    -1.171540      22.58
 H      -3.781191     3.080447    -2.394023      20.01
 C      -0.961483     1.420824     0.100272     -17.69
 O      -0.365830     2.755333     0.448475     142.03
 C      -0.319653     0.209867     0.438012      33.41
 H       0.826637     0.247520     0.716456      23.11
 C      -2.086424    -0.955952    -0.629871     -25.09
 C      -3.022898    -2.336712    -1.110320      56.24
 H      -3.936905    -1.747811    -1.448936      21.80
 O      -2.076706    -3.252073    -1.990652     130.72
 H      -3.003497    -3.976289    -2.169848      14.26
 C      -3.531626    -3.055322     0.264404      86.40
 H      -2.667553    -3.240762     0.838338      23.25
 O      -4.315730    -2.099005     1.135562     273.16
 H      -4.447367    -2.423225     2.122356      26.60
 C      -4.628325    -4.261103    -0.099702      90.68
 O      -4.107906    -5.087563    -1.107879     333.19
 H      -3.248828    -5.651878    -0.820359      23.97
 H      -5.685906    -3.824623    -0.296471      26.02
 H      -4.877412    -4.827079     0.812838      27.73
55
name = lig-etoh-frame_869
 C       2.266315     1.728409    -2.211669      51.07
 H       1.628381     2.399498    -2.747439      21.06
 C       3.437759     1.530312    -0.033722      81.53
 H       3.484462     1.824071     0.947629      21.72
 C       3.872973     0.268051    -0.425419      15.37
 O       4.837805    -0.640714     0.264558     184.99
 C       5.298662     0.035560     1.566623     104.41
 H       4.563390     0.106166     2.398584      27.94
 H       5.679785     0.937002     1.134823      27.66
 H       5.953108    -0.803733     2.011141      26.00
 C       3.601989    -0.157802    -1.719818      31.15
 O       4.337931    -1.266260    -2.156202     151.18
 H       5.293325    -1.409258    -1.616415      21.78
 C       2.772953     0.440565    -2.583143      62.67
 H       2.480642     0.160986    -3.644583      27.19
 C       2.588390     2.181333    -0.948099      46.02
 C       1.915631     3.501980    -0.284249     114.83
 H       2.728314     4.201253    -0.818992      22.43
 O       2.184520     3.673630     1.142336     262.71
 H       2.817178     4.542617     1.234377      25.93
 C       0.417548     3.510787    -0.543309      65.08
 H      -0.019372     3.477286    -1.595991      20.48
 C      -0.323794     5.032356    -0.093794      89.40
 O       0.601279     5.980832    -0.749751     226.39
 H       0.450788     6.020057    -1.682897      31.91
 H      -0.156531     5.281909     0.957318      25.27
 H      -1.417185     5.177070    -0.298571      25.09
 C      -0.818253    -1.049299     0.067181      42.55
 H      -0.499547    -2.007907     0.280788      23.22
 C      -2.878550     0.290126    -0.889519      45.86
 H      -3.724470     0.334672    -1.592260      22.52
 C      -2.262292     1.498935    -0.542176      25.21
 O      -2.739765     2.800657    -0.789327     160.06
 C      -4.214543     3.027605    -1.283171     108.06
 H      -4.996061     2.260607    -0.747215      23.02
 H      -4.425264     4.054508    -1.361103      26.93
 H      -4.091018     2.995242    -2.306209      27.03
 C      -1.015414     1.457261    -0.009515     -29.71
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 O      -0.372968     2.720247     0.517467     131.76
 C      -0.276996     0.165395     0.450653      39.32
 H       0.615144     0.231559     0.961656      26.27
 C      -2.151635    -0.949347    -0.673755     -17.95
 C      -2.925889    -2.272373    -1.087726      75.03
 H      -3.805329    -1.785929    -1.545121      23.67
 O      -2.146413    -3.245668    -1.979528     249.43
 H      -2.854890    -3.740153    -2.059998      25.34
 C      -3.600352    -3.029078     0.261473      84.33
 H      -2.730903    -3.649693     0.839734      21.29
 O      -4.272823    -2.107920     1.119707     319.79
 H      -4.239084    -2.445668     1.963866      31.02
 C      -4.551054    -4.212192    -0.033477      99.05
 O      -4.099373    -5.109133    -1.137091     343.62
 H      -3.345505    -5.589762    -0.863412      28.83
 H      -5.307839    -3.602608    -0.532681      26.12
 H      -4.731487    -5.064707     0.668658      25.56
55
name = lig-etoh-frame_870
 C       2.284354     1.665533    -2.195253      60.36
 H       1.747007     2.353826    -2.908732      21.37
 C       3.387585     1.495995    -0.024720      55.06
 H       3.576947     1.914365     1.037538      19.00
 C       3.902962     0.284658    -0.432207      21.06
 O       4.750972    -0.658933     0.314239     211.91
 C       5.307589     0.005852     1.560751     107.40
 H       4.476935     0.132267     2.301247      27.13
 H       5.759129     1.076842     1.441357      26.64
 H       6.036707    -0.676453     1.901846      28.04
 C       3.614229    -0.250514    -1.769655      23.42
 O       4.327674    -1.276964    -2.218608     156.54
 H       5.219066    -1.405480    -1.700582      23.43
 C       2.729757     0.459164    -2.563836      66.77
 H       2.824652     0.051275    -3.590779      27.49
 C       2.523464     2.241816    -0.843729      56.54
 C       1.834901     3.477581    -0.289541     127.76
 H       2.516137     4.170333    -0.675579      22.79
 O       2.184900     3.633821     1.118774     303.10
 H       2.832799     4.255382     1.166379      31.22
 C       0.356130     3.586436    -0.527268      60.97
 H       0.108049     3.118167    -1.479329      23.52
 C      -0.275435     5.006822    -0.100028      96.62
 O       0.582736     6.038194    -0.730151     206.95
 H       0.524954     5.975340    -1.736367      28.87
 H       0.015713     5.022490     0.986393      23.84
 H      -1.345024     5.261709    -0.297490      24.72
 C      -0.875448    -1.023830     0.070956      26.47
 H      -0.248050    -2.049253    -0.082019      20.71
 C      -2.841435     0.242239    -0.834049      57.03
 H      -3.648279     0.291303    -1.566086      23.78
 C      -2.251181     1.533801    -0.521274      22.68
 O      -2.721543     2.766404    -0.770762     140.30
 C      -4.172058     3.018561    -1.354727      99.24
 H      -5.091663     2.597250    -1.053799      24.69
 H      -4.669631     4.068206    -1.035596      23.44
 H      -4.537036     2.451284    -2.478805      21.44
 C      -0.945224     1.477321    -0.021939      -7.55
 O      -0.380175     2.637358     0.544780     114.62
 C      -0.284554     0.186196     0.417742       4.96
 H       0.526374     0.308679     1.254146      21.97
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 C      -2.203855    -0.968133    -0.697177      18.79
 C      -2.837363    -2.191685    -1.026823      77.83
 H      -3.689281    -2.042060    -1.822210      21.13
 O      -2.223263    -3.187845    -1.932607     154.89
 H      -2.954637    -4.094414    -2.161431      13.88
 C      -3.590721    -3.053157     0.278402      93.53
 H      -2.824207    -3.612854     0.713726      24.86
 O      -4.229355    -2.106369     1.082898     303.21
 H      -4.027868    -2.442434     2.115733      25.10
 C      -4.476076    -4.167114    -0.035961     100.76
 O      -4.096887    -5.110159    -1.186546     293.60
 H      -3.270991    -5.749520    -0.865930      23.82
 H      -5.315980    -3.684198    -0.593817      25.86
 H      -4.789793    -4.790202     0.811501      28.04
55
name = lig-etoh-frame_871
 C       2.260501     1.706573    -2.130934      59.56
 H       1.841905     2.145908    -3.028889      21.97
 C       3.331671     1.469939     0.025920      44.64
 H       3.663236     1.901756     0.932529      21.05
 C       3.947703     0.235200    -0.466456      20.85
 O       4.666296    -0.621585     0.373989     242.35
 C       5.302551    -0.024016     1.538571     108.68
 H       4.406410     0.099614     2.226731      25.42
 H       5.786466     0.964579     1.622339      26.73
 H       6.222977    -0.637727     1.874620      25.85
 C       3.648493    -0.302308    -1.729362      17.09
 O       4.326081    -1.326368    -2.305144     202.29
 H       5.024867    -1.473386    -1.716603      27.39
 C       2.730884     0.432422    -2.598073      52.97
 H       2.874330     0.088226    -3.612086      26.98
 C       2.445484     2.234697    -0.788367      48.76
 C       1.819590     3.456241    -0.279602     107.24
 H       2.030372     4.573106    -0.879887      18.28
 O       2.160108     3.582958     1.106256     277.43
 H       3.070198     4.116213     1.197720      25.80
 C       0.232300     3.648934    -0.480481      55.32
 H       0.168525     2.977094    -1.371666      22.55
 C      -0.167599     4.976745    -0.122213     116.87
 O       0.553957     6.106690    -0.715931     190.41
 H       0.584620     5.767451    -1.757272      25.04
 H       0.012753     4.891797     0.943208      23.81
 H      -1.223844     5.091657    -0.305154      24.83
 C      -0.960800    -1.016006     0.012875      64.72
 H      -0.226776    -1.755045    -0.151887      24.17
 C      -2.814146     0.242176    -0.819265      63.22
 H      -3.759645     0.190017    -1.389807      24.54
 C      -2.226173     1.500797    -0.515935      -3.15
 O      -2.778731     2.768507    -0.775688     130.66
 C      -4.159868     2.988172    -1.452340     111.39
 H      -5.046937     2.436713    -0.729193      23.80
 H      -4.289462     3.947049    -1.062953      25.69
 H      -4.341847     2.507915    -2.262116      27.34
 C      -0.837207     1.460413     0.042133      -3.49
 O      -0.367217     2.569246     0.549191     137.93
 C      -0.332371     0.252855     0.379361      37.32
 H       0.424708     0.299683     1.108173      24.34
 C      -2.147991    -0.979786    -0.652864      34.81
 C      -2.886262    -2.218342    -1.017774      89.08
 H      -3.714031    -1.976362    -1.673326      24.32
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 O      -2.267760    -3.152443    -1.889307     271.42
 H      -2.767591    -3.976226    -1.947826      21.62
 C      -3.486171    -3.049595     0.265023      76.69
 H      -2.473597    -3.394560     0.841695      22.58
 O      -4.188811    -2.109719     1.084992     345.47
 H      -4.006977    -2.133128     2.045485      28.44
 C      -4.477982    -4.151575    -0.129162      94.86
 O      -4.069181    -5.113270    -1.213601     314.79
 H      -3.421021    -5.781663    -0.972683      29.38
 H      -5.528088    -3.889401    -0.417967      26.69
 H      -4.836576    -4.402760     0.949894      26.07
55
name = lig-etoh-frame_872
 C       2.229021     1.725258    -2.096726      61.38
 H       1.738962     2.253796    -2.944476      21.11
 C       3.286038     1.419064     0.043469      57.65
 H       3.700616     1.826966     0.988972      19.99
 C       3.954936     0.208579    -0.467608      30.17
 O       4.617776    -0.573323     0.422373     245.23
 C       5.293639    -0.058532     1.551681     115.64
 H       4.571414    -0.057163     2.379497      26.20
 H       5.722553     0.971951     1.335111      26.38
 H       6.042282    -0.749873     1.846700      26.63
 C       3.642350    -0.300052    -1.719079      28.17
 O       4.325032    -1.391518    -2.394526     144.76
 H       5.022234    -1.848056    -1.602106      22.82
 C       2.792172     0.408774    -2.577934      56.88
 H       2.645528     0.264532    -3.727994      26.77
 C       2.391983     2.170039    -0.792460      38.08
 C       1.791556     3.519268    -0.278349     116.50
 H       1.851871     4.364655    -0.883840      22.86
 O       2.140535     3.561694     1.103742     304.82
 H       3.148887     3.810504     1.272056      26.92
 C       0.194602     3.556198    -0.431523      80.14
 H      -0.094628     3.293321    -1.484903      20.11
 C      -0.105107     4.989271    -0.116777     107.11
 O       0.522383     6.143457    -0.733968     254.06
 H       0.624149     5.893057    -1.596468      33.12
 H      -0.018375     5.077274     1.003851      23.80
 H      -1.246802     4.967596    -0.290132      23.04
 C      -0.958301    -0.961559    -0.036373      77.81
 H      -0.240889    -1.846309    -0.011810      22.26
 C      -2.811501     0.282483    -0.832689      57.29
 H      -3.871540     0.169446    -1.084045      24.78
 C      -2.188096     1.443147    -0.536095      -8.24
 O      -2.844514     2.763534    -0.792522     131.45
 C      -4.149343     2.912915    -1.407269      93.19
 H      -4.568122     2.407115    -0.654229      24.63
 H      -4.020500     4.124516    -1.488089      21.69
 H      -4.047156     2.559023    -2.710879      21.35
 C      -0.849074     1.446595     0.079367      -5.48
 O      -0.321568     2.583711     0.574597     205.14
 C      -0.380199     0.252387     0.350757      86.38
 H       0.612907     0.195719     0.890022      24.95
 C      -2.121704    -1.001088    -0.615044      -7.94
 C      -3.008612    -2.283011    -1.013050      82.08
 H      -4.035875    -1.687856    -1.379467      20.25
 O      -2.242314    -3.115176    -1.857443     216.69
 H      -2.873442    -4.047651    -1.756595      13.33
 C      -3.329721    -3.001282     0.238773      93.77
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 H      -2.497061    -3.267086     0.762927      24.86
 O      -4.163024    -2.100845     1.087403     344.27
 H      -3.950398    -1.997318     2.023379      29.14
 C      -4.513547    -4.158562    -0.196044      93.55
 O      -4.056233    -5.104886    -1.223744     301.81
 H      -3.411679    -5.839653    -0.880002      26.63
 H      -5.507141    -3.785481    -0.459182      27.42
 H      -4.631387    -4.504707     0.830184      27.20
55
name = lig-etoh-frame_873
 C       2.207355     1.673257    -2.120226      46.77
 H       1.577519     2.414959    -2.649981      20.94
 C       3.259017     1.351406     0.024366      53.05
 H       3.549283     1.674430     1.058099      19.94
 C       3.905503     0.236859    -0.417408      29.41
 O       4.593073    -0.569313     0.450246     220.41
 C       5.278357    -0.069733     1.584394     109.08
 H       4.782924    -0.035727     2.636190      24.80
 H       5.652891     0.875322     1.112869      25.39
 H       6.018731    -0.937266     1.757017      24.23
 C       3.651088    -0.326226    -1.784683      26.33
 O       4.330473    -1.457274    -2.429760     216.85
 H       4.773719    -2.072119    -1.910564      29.62
 C       2.825572     0.476198    -2.551952      60.49
 H       2.532252     0.277616    -3.514351      24.71
 C       2.370845     2.119467    -0.799162      34.85
 C       1.749178     3.503805    -0.279025     105.65
 H       2.306537     4.391656    -1.043771      19.84
 O       2.122602     3.566146     1.111510     350.67
 H       3.003255     3.681451     1.231763      30.71
 C       0.243977     3.433475    -0.396234     106.71
 H      -0.300168     3.543602    -1.377586      19.72
 C      -0.149367     5.027656    -0.050852      95.52
 O       0.492135     6.157361    -0.750010     195.96
 H       0.643356     6.058967    -1.827131      27.22
 H       0.026917     5.360638     0.964916      25.51
 H      -1.187297     5.098282    -0.258881      25.90
 C      -0.848443    -0.952362    -0.063833      33.49
 H      -0.469200    -1.970472     0.288019      21.79
 C      -2.823507     0.259463    -0.845499      55.14
 H      -3.921869     0.311968    -0.884726      23.84
 C      -2.171719     1.467800    -0.576058      21.61
 O      -2.834385     2.734301    -0.795402     207.71
 C      -4.056635     2.872311    -1.421339     126.90
 H      -4.908691     2.327473    -0.661940      23.29
 H      -4.253074     3.838972    -1.812173      26.41
 H      -4.039062     2.549505    -2.321212      28.73
 C      -0.963389     1.480023     0.080248       5.06
 O      -0.272544     2.643357     0.603700     199.86
 C      -0.339168     0.194164     0.367127      54.17
 H       0.770344     0.118973     0.540054      24.18
 C      -2.233400    -1.006846    -0.644046      -9.64
 C      -3.093758    -2.242723    -1.001741      94.09
 H      -4.051709    -1.842757    -1.164921      23.21
 O      -2.235169    -3.102399    -1.839468     219.86
 H      -2.759464    -4.025666    -1.795896      16.33
 C      -3.289259    -2.953548     0.225484      77.44
 H      -2.336222    -3.468773     0.766614      20.74
 O      -4.143945    -2.090513     1.071829     286.04
 H      -3.755821    -2.033423     2.105836      25.13
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 C      -4.492421    -4.165788    -0.203717      73.45
 O      -4.046397    -5.099292    -1.232352     261.41
 H      -3.419557    -5.747434    -0.718562      25.20
 H      -5.310356    -3.505777    -0.648329      25.66
 H      -4.542526    -4.929231     0.644540      24.42
55
name = lig-etoh-frame_874
 C       2.175390     1.650029    -2.107642      47.80
 H       1.463633     2.271611    -2.640959      22.27
 C       3.213447     1.330806     0.019090      52.13
 H       3.275732     1.535570     1.059167      19.61
 C       3.847238     0.200158    -0.409848      18.16
 O       4.558965    -0.611997     0.464973     228.09
 C       5.295685    -0.091970     1.622465     122.12
 H       4.826781     0.155166     2.557010      26.93
 H       5.816389     0.844428     1.366115      26.85
 H       6.098103    -0.806727     1.638329      25.89
 C       3.699846    -0.356377    -1.819659      20.94
 O       4.298676    -1.485587    -2.466215     182.76
 H       4.699459    -2.210113    -1.864635      25.66
 C       2.835213     0.556062    -2.560183      59.37
 H       2.529557     0.052605    -3.591655      22.31
 C       2.378890     2.082272    -0.798809      28.86
 C       1.796139     3.419879    -0.322930     123.58
 H       2.368638     4.125596    -0.782047      23.39
 O       2.073261     3.588391     1.114894     293.69
 H       3.145445     3.755275     1.163360      25.51
 C       0.311729     3.468681    -0.366967      83.14
 H      -0.282710     3.327957    -1.314156      21.18
 C      -0.212176     5.083199     0.017711      80.32
 O       0.476777     6.161428    -0.791583     207.22
 H       0.420740     6.017571    -1.792103      28.57
 H       0.081071     5.432909     1.029968      24.44
 H      -1.342432     5.226237    -0.208659      23.87
 C      -0.840723    -1.044846    -0.106812      18.76
 H      -0.529050    -1.940413     0.366339      22.83
 C      -2.858720     0.220209    -0.851377      60.68
 H      -3.921730     0.420335    -0.946489      24.30
 C      -2.196511     1.541245    -0.619238      31.84
 O      -2.766485     2.712257    -0.775633     208.50
 C      -4.027072     2.802115    -1.407578     115.42
 H      -5.029391     2.624812    -1.147886      25.42
 H      -4.459260     3.863735    -1.665255      23.95
 H      -4.108555     1.885996    -2.443281      21.82
 C      -1.021265     1.494207     0.109864      -4.32
 O      -0.266788     2.663752     0.626187     158.80
 C      -0.251286     0.201600     0.365946      18.14
 H       0.806205     0.228283     0.486934      22.80
 C      -2.311023    -0.974648    -0.677744      17.74
 C      -3.068492    -2.163805    -0.979582      69.46
 H      -4.224376    -2.000410    -1.467508      20.81
 O      -2.246982    -3.087034    -1.840402     193.51
 H      -2.684773    -4.021068    -1.936992      17.53
 C      -3.343109    -2.995544     0.283515      98.85
 H      -2.485081    -3.453751     0.606709      25.70
 O      -4.102574    -2.084270     1.077378     359.98
 H      -3.803408    -2.153395     1.943067      32.04
 C      -4.406484    -4.168525    -0.179385      97.16
 O      -4.026082    -5.093957    -1.248143     325.62
 H      -3.415609    -5.682972    -0.842225      30.52
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 H      -5.123786    -3.513004    -0.592099      28.10
 H      -4.856558    -4.894484     0.527227      26.71
55
name = lig-etoh-frame_875
 C       2.126299     1.665548    -2.085000      62.61
 H       1.401820     2.000877    -2.870292      22.46
 C       3.162692     1.321451     0.034703      50.48
 H       3.027767     1.485641     1.172212      19.60
 C       3.817481     0.080728    -0.457875      17.26
 O       4.527965    -0.667471     0.485643     230.77
 C       5.346659    -0.095224     1.622389      86.99
 H       4.618751     0.170404     2.506144      24.61
 H       5.964408     0.879709     1.566593      24.81
 H       6.202847    -0.802976     1.795840      25.43
 C       3.736192    -0.324729    -1.810401      20.12
 O       4.246079    -1.490180    -2.495031     144.57
 H       4.659795    -2.059716    -1.633023      22.23
 C       2.862517     0.521611    -2.630513      49.49
 H       2.663549     0.105835    -3.553721      24.31
 C       2.389384     2.059544    -0.798487      57.25
 C       1.865588     3.287951    -0.317842     125.05
 H       2.436866     4.336827    -0.866265      18.47
 O       2.050898     3.612745     1.112194     292.75
 H       2.992329     3.961642     1.205274      28.14
 C       0.317847     3.618410    -0.355452      57.86
 H       0.012722     3.109135    -1.323254      21.84
 C      -0.254382     5.148664     0.045194      95.29
 O       0.453590     6.148525    -0.832738     243.81
 H       0.204347     5.832907    -1.719597      29.18
 H       0.041106     5.275548     1.098018      25.53
 H      -1.306552     5.155238    -0.029902      26.27
 C      -0.914213    -1.083448    -0.140732      28.70
 H      -0.409772    -2.092987     0.253272      22.28
 C      -2.913336     0.299525    -0.859150      64.85
 H      -3.971380     0.283928    -1.204165      22.98
 C      -2.208523     1.518725    -0.618667       7.38
 O      -2.737448     2.744584    -0.756355     152.52
 C      -4.056104     2.707246    -1.506184     109.03
 H      -5.127313     2.500766    -0.914405      24.05
 H      -3.995792     3.810632    -1.639531      24.29
 H      -3.993659     1.998245    -2.104843      26.62
 C      -0.965734     1.468738     0.162696       5.60
 O      -0.303060     2.639813     0.645902     125.10
 C      -0.237794     0.215475     0.296727     -13.31
 H       0.854060     0.409363     0.720975      19.96
 C      -2.265666    -0.952266    -0.679783      14.05
 C      -3.063021    -2.175161    -0.985228      82.79
 H      -3.805276    -2.083667    -1.706917      23.49
 O      -2.243384    -3.048780    -1.852025     170.11
 H      -2.879896    -3.994944    -2.060835      13.77
 C      -3.460189    -3.066575     0.309161      80.05
 H      -2.383703    -3.424010     0.743005      23.35
 O      -4.062136    -2.083481     1.094152     321.30
 H      -3.963533    -2.240223     2.130262      26.57
 C      -4.326286    -4.170652    -0.146394      97.88
 O      -3.996291    -5.076906    -1.270139     275.55
 H      -3.236641    -5.834736    -1.042362      22.38
 H      -5.243236    -3.591257    -0.584808      25.42
 H      -5.067384    -4.540751     0.669865      26.75
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name = lig-etoh-frame_876
 C       2.112265     1.605407    -2.156622      54.04
 H       1.397496     1.969910    -2.885007      21.40
 C       3.146346     1.228103     0.064154      63.39
 H       3.034798     1.467780     1.062940      23.42
 C       3.796482     0.005473    -0.458979      22.67
 O       4.527653    -0.729930     0.508481     223.38
 C       5.389822    -0.081372     1.625481      86.31
 H       4.641902    -0.056586     2.346776      27.69
 H       5.845432     0.839635     1.353269      27.25
 H       6.002836    -0.906244     2.056893      26.46
 C       3.736112    -0.266843    -1.838705      30.70
 O       4.192787    -1.477475    -2.466370     196.05
 H       4.662148    -1.834594    -1.813073      25.06
 C       2.887182     0.480109    -2.651605      56.34
 H       2.743493     0.211535    -3.786793      24.87
 C       2.386555     2.038332    -0.809998      62.63
 C       1.895955     3.327791    -0.256940     137.88
 H       2.254759     4.053385    -0.911759      25.22
 O       2.058573     3.629629     1.110516     317.60
 H       2.831790     4.120834     1.330321      30.86
 C       0.293565     3.738711    -0.365490      42.45
 H       0.181543     3.265020    -1.378020      21.45
 C      -0.229612     5.166268     0.044447     102.97
 O       0.407675     6.118185    -0.857712     229.21
 H       0.067878     5.665000    -1.813104      25.52
 H       0.047569     5.219801     1.103257      25.61
 H      -1.391065     5.080469     0.040967      24.10
 C      -0.969255    -1.051279    -0.137313      74.58
 H      -0.493830    -1.958821    -0.133525      24.65
 C      -2.948287     0.383736    -0.875766      53.94
 H      -3.848726     0.155178    -1.417753      21.69
 C      -2.191313     1.456130    -0.550825      -8.29
 O      -2.748823     2.787002    -0.744212     109.99
 C      -4.095826     2.691492    -1.523698      86.42
 H      -4.656718     2.378329    -0.689172      23.77
 H      -3.812404     3.652004    -2.036424      22.59
 H      -3.829686     1.800908    -2.550157      21.01
 C      -0.876720     1.416995     0.177967      23.49
 O      -0.357251     2.611987     0.660865     112.30
 C      -0.270827     0.213279     0.211603      30.88
 H       0.547692     0.272386     0.823634      23.06
 C      -2.187600    -0.936861    -0.661140       1.29
 C      -3.019936    -2.254240    -1.002855      64.50
 H      -3.921163    -1.846857    -1.791669      21.79
 O      -2.225519    -3.036954    -1.883352     263.76
 H      -2.846362    -3.656551    -2.013541      25.28
 C      -3.481691    -3.094350     0.299512      93.13
 H      -2.615078    -3.347477     0.809288      26.18
 O      -4.038568    -2.079094     1.152412     300.04
 H      -4.349575    -2.356299     2.138451      26.68
 C      -4.371046    -4.181992    -0.127850      99.57
 O      -3.947261    -5.071022    -1.275158     318.81
 H      -3.259448    -5.709793    -1.111927      27.50
 H      -5.151725    -3.728377    -0.679108      28.10
 H      -4.815808    -4.478299     0.849934      28.34
55
name = lig-etoh-frame_877
 C       2.144733     1.514491    -2.233569      45.63
 H       1.422286     2.149444    -2.802933      21.34
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 C       3.133877     1.100822     0.037578      56.31
 H       3.246539     1.450345     1.148035      20.77
 C       3.787287    -0.001282    -0.388693      19.77
 O       4.553225    -0.808683     0.509330     217.66
 C       5.380396    -0.109241     1.613208      86.02
 H       4.579173     0.064501     2.474683      24.65
 H       5.768910     0.842667     1.073953      25.39
 H       5.953606    -0.929383     2.034759      26.09
 C       3.724648    -0.254632    -1.882643      35.92
 O       4.136550    -1.439243    -2.424169     114.68
 H       4.990374    -1.895566    -1.845677      20.92
 C       2.868223     0.479947    -2.689130      57.19
 H       2.905952     0.323459    -3.755119      25.06
 C       2.367330     1.984507    -0.828935      44.70
 C       1.839932     3.448856    -0.178673      91.26
 H       2.361610     4.116510    -1.154061      19.97
 O       2.091971     3.631707     1.127635     280.13
 H       2.854944     4.348206     1.456157      24.02
 C       0.292650     3.755718    -0.383891      49.08
 H      -0.097269     3.667483    -1.442855      19.92
 C      -0.199930     5.121051     0.041654     112.34
 O       0.333305     6.069421    -0.893456     273.07
 H       0.251745     5.842245    -1.778706      33.85
 H       0.163966     5.421599     1.056089      25.49
 H      -1.259439     5.141214    -0.016600      26.03
 C      -0.966740    -0.963579    -0.122373      60.25
 H      -0.427702    -1.988310    -0.425542      21.55
 C      -2.909797     0.340959    -0.883980      45.57
 H      -3.796266     0.300606    -1.561248      20.94
 C      -2.183603     1.480152    -0.458410      -6.36
 O      -2.751572     2.795681    -0.743702     149.26
 C      -4.015608     2.666723    -1.586530     109.99
 H      -4.635761     2.349008    -0.642067      22.77
 H      -4.309407     3.527765    -2.317975      24.84
 H      -4.036720     2.060919    -2.299536      28.50
 C      -0.858468     1.410702     0.126297      19.19
 O      -0.407941     2.602063     0.666207      93.94
 C      -0.301124     0.160144     0.162211      42.23
 H       0.586034    -0.086801     0.916221      21.12
 C      -2.226971    -0.918041    -0.667907      -2.50
 C      -2.977897    -2.261044    -1.036504      93.17
 H      -3.892846    -1.803570    -1.258400      25.73
 O      -2.179439    -3.028342    -1.920343     177.97
 H      -2.977883    -3.901713    -2.197603      13.58
 C      -3.448883    -3.044950     0.263987      76.42
 H      -2.522027    -3.557541     0.849233      22.63
 O      -4.054783    -2.072801     1.217753     301.76
 H      -4.436031    -2.469293     1.930884      32.34
 C      -4.462809    -4.211524    -0.123894      79.71
 O      -3.911346    -5.053712    -1.263061     277.78
 H      -3.126744    -5.698261    -0.912607      22.60
 H      -5.320644    -3.716649    -0.712332      25.55
 H      -4.576240    -4.887975     0.835122      25.98
55
name = lig-etoh-frame_878
 C       2.151279     1.529467    -2.212530      52.33
 H       1.587890     2.249276    -2.826954      23.40
 C       3.087906     1.066561     0.033630      61.21
 H       3.417417     1.363276     0.985445      22.61
 C       3.811381    -0.036599    -0.367541      17.02
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 O       4.588245    -0.886144     0.491917     237.35
 C       5.292358    -0.145967     1.582586     120.51
 H       4.801282     0.367490     2.368578      27.01
 H       5.813958     0.652346     1.138231      28.73
 H       6.161778    -0.838243     1.846752      25.84
 C       3.711400    -0.278161    -1.843443      38.97
 O       4.121409    -1.432735    -2.372676     154.62
 H       5.051726    -1.740744    -2.126028      24.26
 C       2.871844     0.468478    -2.756587      47.08
 H       2.983324     0.257209    -3.838436      25.43
 C       2.332645     1.907240    -0.842336      36.32
 C       1.771187     3.549091    -0.229089      91.64
 H       2.351599     4.222968    -0.771780      22.09
 O       2.153582     3.644247     1.180305     302.12
 H       2.805127     4.327212     1.318477      28.01
 C       0.296053     3.704045    -0.392606      64.47
 H      -0.338903     3.817460    -1.308448      17.35
 C      -0.164780     5.076558     0.051305      98.40
 O       0.274025     6.053205    -0.919973     213.00
 H       0.367413     5.808916    -1.960257      27.26
 H       0.225863     5.582222     0.928222      23.97
 H      -1.308187     5.150852     0.019786      23.26
 C      -0.968664    -0.965820    -0.171168      40.36
 H      -0.395612    -1.808394    -0.288162      24.27
 C      -2.832193     0.263839    -0.887851      48.67
 H      -3.691283     0.499134    -1.450405      24.48
 C      -2.209743     1.533639    -0.408204      11.37
 O      -2.742439     2.789635    -0.770214     193.76
 C      -3.944089     2.687438    -1.582602     115.80
 H      -4.897685     2.487759    -1.070412      26.53
 H      -4.554107     3.543221    -1.970664      24.85
 H      -4.112632     1.602643    -2.403019      22.53
 C      -0.907650     1.455898     0.054501     -13.29
 O      -0.435505     2.617733     0.648357      94.53
 C      -0.245907     0.121704     0.208758      40.79
 H       0.659970    -0.162464     0.623927      22.91
 C      -2.319562    -0.921572    -0.690815      52.52
 C      -2.930161    -2.209183    -1.003838      89.41
 H      -4.107813    -1.905150    -1.247456      22.11
 O      -2.176416    -3.058304    -1.981155     251.48
 H      -2.556836    -3.811185    -2.160382      27.13
 C      -3.393420    -3.010271     0.265104      83.42
 H      -2.631979    -3.645577     0.629510      24.16
 O      -4.064326    -2.066531     1.233950     230.06
 H      -4.498447    -2.735213     1.970130      26.50
 C      -4.526240    -4.234079    -0.136929      92.63
 O      -3.872916    -5.037835    -1.239680     340.46
 H      -3.177996    -5.583264    -0.775547      26.92
 H      -5.532804    -3.873810    -0.337263      28.69
 H      -4.544814    -5.132502     0.481478      26.98
55
name = lig-etoh-frame_879
 C       2.154543     1.600489    -2.172593      84.00
 H       1.718250     2.263954    -2.916840      26.42
 C       3.054196     1.081775     0.042947      50.83
 H       3.337027     1.498547     1.055256      20.30
 C       3.830431    -0.090321    -0.418371       7.71
 O       4.614559    -0.932309     0.462841     246.03
 C       5.247300    -0.191744     1.516915     122.16
 H       4.779887     0.434384     2.369233      23.92
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 H       5.948690     0.652268     1.051246      25.96
 H       6.104472    -0.742496     1.824769      26.66
 C       3.673026    -0.304288    -1.767083      28.46
 O       4.139350    -1.469029    -2.353729     193.64
 H       5.045533    -1.632590    -2.161377      28.59
 C       2.907367     0.454064    -2.778237      43.01
 H       2.957900     0.133396    -3.888765      22.68
 C       2.285617     1.870811    -0.834299      33.25
 C       1.747159     3.538233    -0.289221      83.75
 H       2.417703     4.572181    -0.577150      19.84
 O       2.193327     3.641808     1.207612     270.95
 H       2.930557     4.295600     1.210958      26.73
 C       0.246093     3.648236    -0.351039      83.67
 H      -0.217374     3.400552    -1.327175      19.42
 C      -0.163968     5.076412     0.058784      98.51
 O       0.235558     6.068421    -0.974318     257.92
 H       0.329443     5.519804    -1.853102      27.49
 H       0.259230     5.476284     1.007438      23.83
 H      -1.241658     5.011986     0.222731      24.20
 C      -0.984391    -0.995717    -0.239654      21.44
 H      -0.366034    -1.995507    -0.042367      22.34
 C      -2.786852     0.316186    -0.884184      55.38
 H      -3.845799     0.399957    -1.287213      23.67
 C      -2.251358     1.526793    -0.422802      23.76
 O      -2.754874     2.778855    -0.811577     200.23
 C      -3.955838     2.654503    -1.598247     115.31
 H      -4.986742     2.365685    -1.122932      25.54
 H      -4.089261     3.854703    -1.738133      23.54
 H      -3.813304     2.018509    -2.270133      29.53
 C      -0.932464     1.483066     0.029541     -13.63
 O      -0.428190     2.666220     0.596699     152.43
 C      -0.224066     0.147710     0.255383      20.46
 H       0.950594     0.070577     0.405630      19.89
 C      -2.309403    -0.981715    -0.693821      47.56
 C      -2.991781    -2.194181    -0.980488      96.63
 H      -3.820956    -2.150440    -1.631443      23.08
 O      -2.158571    -3.037887    -2.024101     124.64
 H      -2.602781    -4.103364    -2.042181      15.80
 C      -3.404975    -3.013892     0.278286      76.75
 H      -2.480234    -3.638520     0.682648      21.64
 O      -4.061166    -2.094843     1.223438     254.60
 H      -4.365110    -2.707481     1.971990      27.21
 C      -4.520896    -4.258969    -0.158367      87.82
 O      -3.857471    -5.004227    -1.232831     335.03
 H      -3.221720    -5.600309    -0.805421      28.70
 H      -5.643935    -4.014554    -0.147744      26.57
 H      -4.669212    -5.070901     0.643904      27.35
55
name = lig-etoh-frame_880
 C       2.199002     1.621045    -2.212985      92.90
 H       1.724485     2.345584    -2.950796      23.94
 C       3.070669     1.091589     0.064605      62.53
 H       3.046457     1.608689     1.047709      15.14
 C       3.805135    -0.080866    -0.421947      17.35
 O       4.619870    -0.947257     0.409376     235.54
 C       5.279857    -0.179285     1.439254     110.35
 H       4.538738     0.107177     2.187143      25.17
 H       5.781772     0.587799     0.950025      27.93
 H       5.930409    -0.949138     2.038251      24.94
 C       3.617819    -0.363728    -1.779080      14.89
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 O       4.165455    -1.528382    -2.352449     120.37
 H       5.235512    -1.629381    -1.981628      22.59
 C       2.928721     0.479000    -2.701077      34.15
 H       2.898763     0.134479    -3.686053      19.40
 C       2.245350     1.923439    -0.793298      79.74
 C       1.806405     3.475602    -0.287454     104.26
 H       2.117028     4.310446    -0.794865      24.92
 O       2.196784     3.624611     1.194103     290.84
 H       3.218836     4.103968     1.201700      25.68
 C       0.183356     3.596556    -0.310239      89.04
 H       0.104668     3.072782    -1.324348      18.53
 C      -0.180355     5.093985     0.065325      94.82
 O       0.195127     6.062869    -1.020893     302.86
 H       0.230610     5.507374    -1.792697      30.48
 H       0.341028     5.194051     1.036670      24.81
 H      -1.276233     5.004645     0.328720      24.30
 C      -0.916585    -1.038210    -0.252532      46.69
 H      -0.626105    -2.013977     0.090372      22.88
 C      -2.835505     0.369634    -0.889664      58.07
 H      -3.858082     0.200065    -1.083114      23.86
 C      -2.261033     1.508349    -0.479136      15.09
 O      -2.776164     2.745502    -0.826491     164.92
 C      -3.997039     2.723488    -1.573993      97.03
 H      -4.735506     2.200903    -0.988353      24.91
 H      -3.771003     3.739268    -1.859508      23.01
 H      -3.489726     2.228033    -2.805985      21.79
 C      -0.904195     1.462521     0.062272     -14.36
 O      -0.401143     2.722550     0.539118     190.73
 C      -0.259452     0.208656     0.244806      43.72
 H       0.790286     0.407378     0.263668      19.95
 C      -2.228666    -0.987304    -0.684025      -3.15
 C      -3.082512    -2.265137    -1.020605      72.74
 H      -3.829478    -2.089665    -1.894867      19.43
 O      -2.143452    -3.037626    -2.041808     195.59
 H      -2.671707    -3.869177    -1.754102      17.60
 C      -3.467418    -3.066915     0.292260      87.49
 H      -2.518938    -3.350983     0.749642      22.94
 O      -4.042841    -2.142843     1.193628     333.72
 H      -4.203086    -2.497046     2.045120      29.87
 C      -4.471299    -4.293001    -0.121358      91.14
 O      -3.870553    -4.965855    -1.239850     324.05
 H      -3.235792    -5.776787    -0.927369      24.29
 H      -5.476592    -3.954729    -0.473273      27.26
 H      -4.570150    -4.723718     0.910280      27.54
55
name = lig-etoh-frame_881
 C       2.258157     1.641739    -2.242732      35.88
 H       1.764520     2.292463    -2.899046      20.51
 C       3.076377     1.124239     0.070734      63.06
 H       2.996177     1.459754     1.094017      17.50
 C       3.749438    -0.035028    -0.381965      13.69
 O       4.608202    -0.943021     0.320587     220.04
 C       5.306541    -0.208595     1.397395     108.73
 H       4.359926    -0.012903     1.983953      24.48
 H       5.804502     0.754818     0.959356      26.05
 H       5.738408    -0.946924     2.007950      26.61
 C       3.580217    -0.447111    -1.824175      13.69
 O       4.221129    -1.584157    -2.345541     209.50
 H       4.972177    -1.754395    -1.835620      26.62
 C       2.925856     0.516750    -2.577507      53.08
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 H       2.836823     0.170143    -3.714751      20.05
 C       2.253186     2.011702    -0.781137      47.39
 C       1.847424     3.346963    -0.211609     100.45
 H       2.041852     4.050527    -1.275503      18.32
 O       2.212622     3.609107     1.134893     356.25
 H       3.127367     3.762246     1.289901      31.69
 C       0.213498     3.561932    -0.344541      74.25
 H       0.112781     3.284178    -1.380439      17.60
 C      -0.209625     5.073501     0.048850      91.66
 O       0.148971     6.043247    -1.017691     257.82
 H       0.118094     5.580847    -2.047181      23.80
 H       0.475719     5.159047     0.918599      24.28
 H      -1.290547     5.228295     0.286006      24.02
 C      -0.841394    -1.047414    -0.213116      58.69
 H      -0.545747    -2.084227     0.109202      21.32
 C      -2.904003     0.293721    -0.885791      50.82
 H      -4.029474     0.218155    -1.057934      22.25
 C      -2.219836     1.521072    -0.542640       7.64
 O      -2.777306     2.706435    -0.802247     194.90
 C      -3.944654     2.781753    -1.626202     112.25
 H      -4.720755     2.203639    -1.088236      25.26
 H      -4.203607     3.963332    -2.019612      23.25
 H      -3.839370     2.461090    -2.486089      29.74
 C      -0.912360     1.448564     0.097835      23.89
 O      -0.399984     2.722323     0.536313     186.53
 C      -0.321471     0.270429     0.186290      47.07
 H       0.769257     0.428732     0.400549      19.04
 C      -2.183887    -0.939170    -0.689977     -24.07
 C      -3.115706    -2.301410    -1.112741      56.35
 H      -4.019325    -1.843972    -1.609199      22.60
 O      -2.149816    -3.044511    -2.004924     193.82
 H      -2.617527    -3.964563    -1.845981      16.29
 C      -3.543568    -3.113000     0.264720      82.47
 H      -2.517977    -3.384220     0.721284      21.15
 O      -4.046514    -2.176853     1.151438     310.20
 H      -3.943309    -2.235711     2.278150      23.93
 C      -4.396001    -4.275766    -0.049084      92.48
 O      -3.879694    -4.967401    -1.241594     327.72
 H      -3.343749    -5.733917    -1.112222      28.63
 H      -5.203869    -3.815570    -0.675340      24.72
 H      -4.511701    -4.754855     0.930402      26.96
55
name = lig-etoh-frame_882
 C       2.301775     1.713694    -2.159253      22.49
 H       1.778010     2.274873    -3.040601      18.59
 C       3.055500     1.177028     0.062401      56.76
 H       3.159002     1.201200     1.210481      17.95
 C       3.687847    -0.027508    -0.407950      29.58
 O       4.602985    -0.912351     0.216100     242.03
 C       5.263643    -0.238906     1.359264     114.85
 H       4.469011     0.218011     1.972845      26.83
 H       5.874531     0.646727     1.223336      28.51
 H       5.936173    -0.973724     1.932700      26.40
 C       3.574297    -0.503679    -1.784207       7.86
 O       4.249185    -1.619445    -2.343724     165.56
 H       4.911017    -1.963287    -1.568329      23.21
 C       2.915560     0.485560    -2.558344      65.07
 H       2.846704     0.353183    -3.561186      23.57
 C       2.332649     2.036345    -0.804093      37.26
 C       1.832065     3.250980    -0.209733     124.12
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 H       2.238021     3.824146    -0.965063      20.11
 O       2.202527     3.593170     1.059322     319.09
 H       3.274342     3.576545     1.291800      25.84
 C       0.302777     3.569910    -0.410404      55.86
 H      -0.145305     3.563006    -1.482717      17.56
 C      -0.206659     5.031313    -0.004963     102.17
 O       0.107149     6.014556    -1.016186     283.45
 H       0.041813     5.752897    -1.879834      32.65
 H       0.455198     5.424962     0.797630      24.39
 H      -1.244735     5.252229     0.264570      24.08
 C      -0.825971    -1.005567    -0.162684      48.64
 H      -0.185694    -1.955233    -0.002912      19.70
 C      -2.935842     0.207013    -0.857756      53.67
 H      -3.941298     0.333807    -1.141839      19.94
 C      -2.195666     1.477007    -0.611137       6.11
 O      -2.771820     2.716954    -0.775628     188.93
 C      -3.924573     2.880825    -1.645401     103.07
 H      -4.891841     2.435387    -1.282337      24.06
 H      -4.493908     3.865274    -1.690192      23.40
 H      -3.983480     2.147394    -2.861834      20.37
 C      -1.003617     1.510696     0.089522      28.16
 O      -0.430431     2.663300     0.578048     174.36
 C      -0.300641     0.245898     0.135644      13.91
 H       0.661943     0.184066     0.746552      18.40
 C      -2.194665    -0.938089    -0.712906      12.63
 C      -3.073095    -2.273281    -1.157808      63.83
 H      -4.067016    -1.853422    -1.427336      23.35
 O      -2.197629    -3.059045    -1.935262     191.57
 H      -2.435711    -4.101667    -2.256437      17.17
 C      -3.502940    -3.113904     0.224639      90.16
 H      -2.558687    -3.631895     0.522802      23.40
 O      -4.086881    -2.177636     1.143233     371.68
 H      -3.711551    -2.168377     1.980437      31.74
 C      -4.346034    -4.247619    -0.010649      96.35
 O      -3.888946    -4.987831    -1.249819     309.02
 H      -3.261425    -5.803404    -1.054630      26.16
 H      -5.307746    -3.741329    -0.389697      25.57
 H      -4.689448    -5.062460     0.720445      26.36
55
name = lig-etoh-frame_883
 C       2.346828     1.750717    -2.101787      35.37
 H       1.917938     2.279036    -2.863406      17.77
 C       3.070126     1.158957     0.068941      48.36
 H       3.206799     1.260658     1.075478      19.83
 C       3.638023    -0.049786    -0.485320      25.63
 O       4.617878    -0.847410     0.147303     243.07
 C       5.216473    -0.277173     1.352878     124.97
 H       4.631162     0.234907     2.142438      27.39
 H       6.004505     0.554148     1.118347      26.98
 H       5.933482    -0.985860     1.738336      27.88
 C       3.563068    -0.508088    -1.736243      22.63
 O       4.267544    -1.627336    -2.318917     155.39
 H       4.684386    -2.180372    -1.486582      22.20
 C       2.895971     0.444034    -2.574020     105.31
 H       2.898870     0.392416    -3.767600      29.06
 C       2.430491     1.996629    -0.794432      26.44
 C       1.780010     3.228264    -0.275933     133.58
 H       2.563330     4.162860    -0.723885      19.16
 O       2.194178     3.572570     1.034783     314.18
 H       3.153367     3.627445     0.984945      28.83
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 C       0.346858     3.600778    -0.456445      51.54
 H      -0.196370     3.470810    -1.362130      20.61
 C      -0.150897     5.011384    -0.050269      96.26
 O       0.078526     6.013872    -1.001893     232.09
 H      -0.044741     5.652009    -2.031207      25.93
 H       0.288879     5.539044     0.815958      23.76
 H      -1.267264     4.866248     0.270392      22.58
 C      -0.862003    -0.953026    -0.150432      45.30
 H      -0.109270    -1.700727    -0.162236      21.01
 C      -2.903152     0.199408    -0.825113      51.68
 H      -3.921067     0.291278    -1.312299      19.58
 C      -2.234232     1.411803    -0.670872      13.57
 O      -2.794049     2.758981    -0.775459     190.35
 C      -3.962033     2.903116    -1.713017     114.21
 H      -4.880435     2.413556    -1.246108      24.82
 H      -4.280272     4.047259    -1.352772      22.43
 H      -3.830203     2.494571    -2.507976      29.24
 C      -1.059498     1.524505     0.055070       1.45
 O      -0.461794     2.609203     0.613851     121.15
 C      -0.251950     0.221128     0.148860      11.49
 H       0.513012     0.095422     0.853320      20.00
 C      -2.223634    -1.032093    -0.742403      33.05
 C      -3.006279    -2.240474    -1.105014      82.91
 H      -4.030001    -2.034892    -1.640146      21.97
 O      -2.222497    -3.087182    -1.909309     286.66
 H      -2.644897    -3.779871    -2.240462      27.27
 C      -3.369772    -3.076014     0.198507      85.57
 H      -2.418882    -3.596214     0.528672      22.61
 O      -4.133223    -2.176067     1.114410     323.61
 H      -3.538036    -2.187872     1.940063      27.10
 C      -4.392729    -4.271863    -0.044326     100.29
 O      -3.902323    -5.025149    -1.259458     340.77
 H      -3.245113    -5.663957    -0.831618      27.20
 H      -5.458192    -3.868656    -0.074393      26.63
 H      -4.643148    -5.080227     0.604581      27.41
55
name = lig-etoh-frame_884
 C       2.426317     1.668786    -2.133131      30.95
 H       1.938863     2.544710    -2.776485      15.71
 C       3.126092     1.062847     0.071609      57.14
 H       3.222190     1.510343     1.158830      17.64
 C       3.633987    -0.065675    -0.484704      27.39
 O       4.636525    -0.771289     0.131358     210.78
 C       5.226013    -0.286844     1.339757     115.96
 H       4.639455     0.006483     2.265036      25.85
 H       5.893958     0.412643     0.852880      26.58
 H       5.784761    -1.219642     1.669781      26.45
 C       3.523877    -0.498363    -1.814844      18.45
 O       4.254612    -1.614348    -2.267076     234.12
 H       4.537452    -2.152239    -1.637608      29.88
 C       2.866076     0.440066    -2.637941      83.55
 H       2.961126     0.266045    -3.649056      31.23
 C       2.479419     1.988214    -0.744369      64.55
 C       1.811920     3.318826    -0.366515     121.87
 H       2.222128     4.120389    -0.817878      25.14
 O       2.167130     3.539652     1.052545     304.04
 H       3.138842     3.807813     0.914624      27.95
 C       0.340711     3.621018    -0.460691      33.02
 H      -0.078279     3.166934    -1.426793      19.10
 C      -0.114462     4.994474    -0.045474     107.44
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 O       0.051598     6.028728    -1.029628     290.26
 H      -0.008461     5.559204    -1.919930      28.22
 H       0.216383     5.322527     0.953496      25.19
 H      -1.117754     4.562514     0.084145      21.95
 C      -0.939564    -0.942276    -0.192545      42.58
 H      -0.168696    -1.855146    -0.290555      19.74
 C      -2.882288     0.196033    -0.840844      57.18
 H      -3.812816     0.103270    -1.369105      20.41
 C      -2.292072     1.433783    -0.689280       5.62
 O      -2.833687     2.774400    -0.801737     160.95
 C      -4.016424     2.964859    -1.634603      85.77
 H      -4.753262     2.252820    -1.238273      22.78
 H      -3.985600     4.050104    -1.584880      23.12
 H      -3.534156     2.756584    -3.005644      20.22
 C      -1.015063     1.437210     0.023974       3.40
 O      -0.485066     2.586925     0.625710      74.09
 C      -0.277503     0.276351     0.195384      25.22
 H       0.684410     0.207945     0.889040      17.97
 C      -2.222662    -1.083176    -0.746096      31.31
 C      -2.973919    -2.261792    -1.033261      96.19
 H      -3.792057    -2.071252    -1.706654      22.31
 O      -2.199459    -3.108223    -1.913645     189.15
 H      -3.157323    -3.741389    -2.166498      15.68
 C      -3.287626    -3.050765     0.188939      78.16
 H      -2.304145    -3.288508     0.734881      21.68
 O      -4.145696    -2.191692     1.081975     300.29
 H      -3.617426    -2.076339     2.038475      23.81
 C      -4.437819    -4.300488    -0.115804      78.39
 O      -3.938881    -5.059160    -1.259360     314.52
 H      -3.241284    -5.591501    -0.861313      26.84
 H      -5.515148    -3.925891    -0.098460      26.21
 H      -4.282335    -4.990750     0.865567      25.07
55
name = lig-etoh-frame_885
 C       2.477043     1.621760    -2.171042      36.44
 H       2.138574     2.439698    -2.707057      17.99
 C       3.153833     1.036567     0.119195      69.33
 H       3.354270     1.427936     1.061104      22.02
 C       3.676531    -0.102718    -0.463406      18.39
 O       4.643055    -0.738241     0.139382     208.93
 C       5.274239    -0.325163     1.327716     117.16
 H       4.564470    -0.100473     2.120738      27.02
 H       5.941191     0.533533     1.004800      27.05
 H       5.703136    -1.292423     1.627022      26.38
 C       3.480252    -0.484706    -1.899294      27.17
 O       4.203932    -1.567909    -2.252656     157.86
 H       4.577898    -2.198699    -1.419772      20.72
 C       2.855721     0.423214    -2.724052      72.04
 H       2.914747     0.145768    -3.845678      23.93
 C       2.490903     1.983986    -0.763962      74.43
 C       1.872222     3.392244    -0.385238      91.57
 H       2.049689     4.290886    -1.356512      20.12
 O       2.148524     3.513184     1.065588     288.07
 H       3.073749     4.073742     1.239653      25.41
 C       0.326330     3.556462    -0.457657      61.04
 H       0.081493     3.140382    -1.432128      16.65
 C      -0.121396     4.955173    -0.031795      91.34
 O       0.030021     6.043175    -1.047992     278.80
 H       0.103591     5.577209    -1.933559      28.39
 H       0.270250     5.082289     0.993624      23.81
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 H      -1.264728     4.734533    -0.068560      19.50
 C      -0.945714    -0.986331    -0.247756      62.27
 H      -0.504158    -1.904068    -0.232439      23.14
 C      -2.894237     0.178796    -0.911161      50.93
 H      -3.884349     0.036985    -1.384345      21.50
 C      -2.318475     1.501352    -0.656546      -5.57
 O      -2.860470     2.753318    -0.828352     213.48
 C      -3.989086     3.001488    -1.608944     128.71
 H      -4.831609     2.323462    -1.443821      25.43
 H      -4.122469     4.218656    -1.860392      22.06
 H      -3.778979     3.044864    -2.505442      28.39
 C      -0.961829     1.391213    -0.006518      -9.92
 O      -0.494806     2.591544     0.605448     103.31
 C      -0.330498     0.278496     0.257855      73.80
 H       0.626153     0.398315     0.574103      21.23
 C      -2.191009    -1.011965    -0.712622      29.93
 C      -2.932911    -2.308972    -0.999861      71.52
 H      -3.881523    -1.863517    -1.586479      20.56
 O      -2.193919    -3.170475    -1.944521     258.79
 H      -2.957054    -3.791101    -2.081266      19.29
 C      -3.306888    -3.034227     0.233181      85.52
 H      -2.394412    -3.187488     0.799506      22.14
 O      -4.133555    -2.208010     1.063451     377.60
 H      -3.946040    -2.035874     1.915083      31.58
 C      -4.389407    -4.328810    -0.125817      95.30
 O      -4.008793    -5.092286    -1.261823     321.28
 H      -3.135156    -5.674643    -1.083832      24.34
 H      -5.385433    -3.954003    -0.342258      27.72
 H      -4.118661    -4.682101     0.794299      27.04
55
name = lig-etoh-frame_886
 C       2.496405     1.633792    -2.168865      60.07
 H       2.207332     2.413687    -3.001020      18.68
 C       3.139640     1.075804     0.128915      78.83
 H       3.545412     1.284612     1.190729      22.12
 C       3.686358    -0.090601    -0.493214      15.62
 O       4.678784    -0.781276     0.148157     234.40
 C       5.329793    -0.364946     1.320851     116.24
 H       4.467301    -0.049386     2.004755      24.16
 H       5.996575     0.544498     1.490466      27.84
 H       5.928537    -1.218059     1.674345      26.27
 C       3.461004    -0.466309    -1.879162      20.77
 O       4.150043    -1.558111    -2.264563     187.30
 H       4.579218    -1.851582    -1.380278      21.73
 C       2.868594     0.372676    -2.844151      36.42
 H       2.734841     0.219338    -3.923735      20.55
 C       2.502765     1.968957    -0.836781     102.22
 C       1.926620     3.433238    -0.392712     128.22
 H       2.158390     4.064307    -1.150612      27.44
 O       2.142145     3.529860     1.070269     390.41
 H       2.873537     3.977601     1.347709      33.26
 C       0.325995     3.442121    -0.435797      71.84
 H       0.004794     3.253869    -1.494479      15.85
 C      -0.202313     4.898691    -0.058748      83.77
 O       0.023763     6.049463    -1.035517     253.43
 H       0.304639     5.639396    -2.021537      24.80
 H       0.329046     5.116853     0.891741      24.04
 H      -1.256378     5.078170     0.073987      22.87
 C      -0.866892    -1.004678    -0.254747      42.48
 H      -0.527513    -2.143424    -0.010254      18.27
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 C      -2.925900     0.235421    -1.003711      50.88
 H      -3.973158     0.156300    -1.344503      21.64
 C      -2.320440     1.494427    -0.610535      10.41
 O      -2.862212     2.734626    -0.829900     205.20
 C      -3.985788     3.070081    -1.589964     102.67
 H      -5.010259     2.584809    -1.541582      24.38
 H      -4.411124     4.135183    -1.455064      23.65
 H      -3.756218     2.846078    -2.983970      21.12
 C      -1.001881     1.471115    -0.043397      -6.18
 O      -0.476115     2.614406     0.547975     189.09
 C      -0.378172     0.161378     0.282463      31.18
 H       0.783524     0.423144     0.402769      16.59
 C      -2.201103    -0.931813    -0.699387      17.49
 C      -2.897349    -2.293456    -1.022977      72.00
 H      -3.863205    -1.970629    -1.322838      23.28
 O      -2.184878    -3.231597    -1.964045     207.75
 H      -2.807954    -4.120342    -2.180946      15.70
 C      -3.379813    -3.032860     0.291655      86.95
 H      -2.427879    -3.476665     0.846388      20.57
 O      -4.151764    -2.206882     1.024065     325.35
 H      -4.041089    -2.136701     2.100274      23.63
 C      -4.258681    -4.306762    -0.113858      84.77
 O      -4.064964    -5.150508    -1.281489     307.98
 H      -3.290851    -5.708888    -1.207147      28.83
 H      -5.299161    -3.872603    -0.471516      24.97
 H      -4.339523    -4.896024     0.949930      25.09
55
name = lig-etoh-frame_887
 C       2.492274     1.649713    -2.258118      66.67
 H       2.194985     2.338040    -3.037623      22.06
 C       3.133638     1.111804     0.084334      62.73
 H       3.486227     1.292264     1.111654      21.78
 C       3.668538    -0.007125    -0.516763      10.21
 O       4.743877    -0.863410     0.132640     227.57
 C       5.363534    -0.384839     1.375949     121.90
 H       4.576898    -0.225529     2.078596      26.40
 H       5.989727     0.518175     1.473724      28.44
 H       6.085425    -1.158077     1.763849      26.13
 C       3.460418    -0.445055    -1.855734      25.42
 O       4.102811    -1.576673    -2.279340     221.63
 H       4.700990    -1.748607    -1.532412      24.44
 C       2.871717     0.371168    -2.874830      29.88
 H       2.665134     0.248949    -3.938890      20.48
 C       2.519852     1.987913    -0.869068      66.67
 C       1.931506     3.354898    -0.339562     121.52
 H       2.605240     4.317006    -0.973016      19.68
 O       2.099225     3.552710     1.058372     347.36
 H       3.152965     3.943320     1.249894      23.34
 C       0.302028     3.382121    -0.435816      87.40
 H      -0.114535     3.247931    -1.458072      16.73
 C      -0.270845     4.873303    -0.102428      81.85
 O       0.044821     6.037922    -1.022593     295.63
 H       0.267659     5.711170    -1.837926      33.46
 H       0.350614     5.269589     0.723565      22.97
 H      -1.339621     5.077687     0.348664      22.84
 C      -0.815133    -1.060914    -0.225104      35.64
 H      -0.411476    -1.928030     0.096696      20.21
 C      -2.936488     0.315962    -1.069079      55.33
 H      -3.969482     0.345369    -1.344004      22.40
 C      -2.324608     1.458997    -0.588281      17.55
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 O      -2.865328     2.739379    -0.812905     206.77
 C      -4.020618     3.128103    -1.686466     112.69
 H      -4.924559     2.532335    -1.379535      25.60
 H      -4.322049     4.007009    -0.900730      21.19
 H      -3.815037     2.904908    -2.570324      28.61
 C      -1.065088     1.499901    -0.048626      -1.09
 O      -0.430624     2.636584     0.468671     237.79
 C      -0.365487     0.128365     0.262089      16.72
 H       0.656532     0.143246     0.494266      18.58
 C      -2.228860    -0.914389    -0.738699       3.18
 C      -2.878940    -2.278011    -1.036079      60.67
 H      -4.008459    -2.160771    -1.441655      20.16
 O      -2.178720    -3.266606    -1.974009     166.71
 H      -2.673880    -4.279351    -2.097077      14.37
 C      -3.374039    -3.102115     0.315061      97.35
 H      -2.603065    -3.588629     0.852300      22.67
 O      -4.203693    -2.164924     1.026787     309.48
 H      -4.019984    -2.495401     1.992014      24.26
 C      -4.179443    -4.282703    -0.065416     119.63
 O      -4.104584    -5.212183    -1.311794     287.74
 H      -3.360816    -5.881572    -1.087858      27.70
 H      -5.092482    -3.801275    -0.272713      28.04
 H      -4.626799    -5.002483     0.572653      28.02
55
name = lig-etoh-frame_888
 C       2.474048     1.654078    -2.370735      55.97
 H       2.040668     2.472409    -3.007613      19.69
 C       3.137462     1.152732     0.004531      58.17
 H       3.279970     1.499712     1.026354      20.22
 C       3.701711     0.030166    -0.524852      13.00
 O       4.800923    -0.926078     0.110351     160.84
 C       5.393507    -0.409215     1.446977     108.89
 H       4.647875    -0.454668     2.338612      24.25
 H       5.870053     0.578160     1.069571      25.88
 H       6.067710    -1.199043     1.736144      26.43
 C       3.474403    -0.428059    -1.876459      25.05
 O       4.052924    -1.612242    -2.287007     148.21
 H       5.047478    -1.861789    -1.789173      21.04
 C       2.862647     0.428708    -2.803441      44.73
 H       2.747420     0.116541    -3.920569      23.69
 C       2.529801     2.031420    -0.893362      63.69
 C       1.930321     3.284299    -0.303874     130.57
 H       2.454485     4.106182    -0.645510      18.03
 O       2.092866     3.587062     1.063260     374.20
 H       3.026271     3.638571     0.983660      28.66
 C       0.265761     3.439020    -0.501520      65.51
 H      -0.050562     3.079219    -1.487315      17.81
 C      -0.292636     4.908336    -0.114973      89.41
 O       0.059051     6.019799    -0.988645     275.21
 H       0.159966     5.591509    -2.030037      24.29
 H       0.338773     5.207369     0.735564      22.94
 H      -1.289147     4.718874     0.251164      23.80
 C      -0.881781    -1.068146    -0.202854      13.91
 H      -0.213239    -2.022178     0.109024      18.59
 C      -2.908485     0.316573    -1.091388      55.45
 H      -3.973351     0.435505    -1.458341      23.63
 C      -2.348964     1.495540    -0.608410      10.67
 O      -2.863051     2.753179    -0.787640     164.88
 C      -4.084783     3.152273    -1.617910      80.06
 H      -4.736164     2.309351    -1.341377      24.17
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 H      -4.128146     4.079625    -1.166011      24.50
 H      -3.726416     3.206407    -3.029995      20.52
 C      -1.049676     1.421119     0.000246       4.29
 O      -0.394723     2.617021     0.416080     206.36
 C      -0.347271     0.195969     0.207947      20.81
 H       0.674824     0.052908     0.797195      16.13
 C      -2.238131    -0.962803    -0.816290      -2.04
 C      -2.934540    -2.323216    -1.047646      81.17
 H      -3.787359    -2.197833    -1.627656      21.21
 O      -2.156820    -3.277367    -1.971353     220.91
 H      -2.746449    -4.049544    -1.879200      19.57
 C      -3.301068    -3.157057     0.296005      74.10
 H      -2.423224    -3.397848     1.093366      19.66
 O      -4.243707    -2.148367     1.051673     254.55
 H      -4.173949    -2.478565     1.930478      25.60
 C      -4.217153    -4.306226    -0.070269      95.39
 O      -4.104903    -5.261465    -1.336478     240.05
 H      -3.554632    -6.020594    -0.887530      26.03
 H      -5.181605    -3.615287    -0.259247      24.85
 H      -4.620538    -5.123417     0.645552      25.98
55
name = lig-etoh-frame_889
 C       2.424765     1.735974    -2.399113      14.79
 H       1.864255     2.502465    -3.042090      13.15
 C       3.160226     1.207969    -0.068007      59.77
 H       3.065504     1.652436     1.004785      16.26
 C       3.804743    -0.029852    -0.540209      20.37
 O       4.819291    -0.950582     0.107352     184.64
 C       5.399037    -0.441726     1.469172     115.20
 H       4.771947    -0.418909     2.322370      27.93
 H       5.683096     0.485569     1.099342      29.04
 H       6.231268    -1.212958     1.594655      26.54
 C       3.530252    -0.419080    -1.864638      35.90
 O       4.027646    -1.660854    -2.299399     216.75
 H       4.878012    -1.813981    -2.095685      26.90
 C       2.859480     0.462223    -2.752384      48.34
 H       2.877288     0.070353    -3.699444      29.43
 C       2.524665     2.052285    -0.969806      51.99
 C       1.844261     3.237730    -0.303115     110.84
 H       2.300576     4.289966    -0.954561      17.18
 O       2.093837     3.590316     1.088349     320.67
 H       3.147594     3.600772     1.194365      28.57
 C       0.261103     3.532223    -0.603273      49.76
 H       0.111562     3.064177    -1.626126      16.45
 C      -0.250583     4.930138    -0.109985      91.65
 O       0.064108     5.985058    -0.991290     323.72
 H      -0.065024     5.654618    -1.872743      31.02
 H       0.181187     5.018304     0.915867      25.18
 H      -1.364474     4.535593    -0.087787      21.22
 C      -0.991429    -1.026532    -0.183961      36.98
 H      -0.416587    -1.911687    -0.129518      18.76
 C      -2.877815     0.262497    -1.089101      49.18
 H      -3.807707     0.271287    -1.612517      20.82
 C      -2.343965     1.532924    -0.647314      -3.59
 O      -2.857778     2.789153    -0.766327     193.32
 C      -4.070062     3.126888    -1.568909     113.51
 H      -4.840546     2.336199    -1.501145      24.00
 H      -4.268328     4.362566    -1.581232      21.86
 H      -3.921364     3.374376    -2.573950      25.21
 C      -1.000520     1.357686     0.049655      -0.97
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 O      -0.379580     2.560853     0.408149     148.68
 C      -0.321802     0.228758     0.157838      44.14
 H       0.431607     0.267075     0.949345      15.73
 C      -2.218981    -1.043480    -0.883533      13.26
 C      -2.964258    -2.388288    -1.059838      69.85
 H      -3.893308    -2.109518    -1.782004      20.34
 O      -2.125229    -3.266033    -1.949129     172.12
 H      -2.949552    -4.078825    -1.767512      14.04
 C      -3.221852    -3.152991     0.294971      72.64
 H      -2.407033    -3.131470     0.911788      21.94
 O      -4.255991    -2.164488     1.050408     242.61
 H      -4.364153    -2.310077     2.168069      24.19
 C      -4.353625    -4.363665    -0.099321      91.57
 O      -4.085501    -5.289081    -1.328332     266.03
 H      -3.673766    -6.031825    -0.930167      30.00
 H      -5.149253    -3.794779    -0.356976      30.91
 H      -4.336174    -4.900334     0.856634      26.63
55
name = lig-etoh-frame_890
 C       2.357412     1.831809    -2.375323      47.29
 H       1.852573     2.379614    -3.121432      15.29
 C       3.217592     1.225801    -0.128729      44.57
 H       3.118499     1.495141     0.851136      15.88
 C       3.925112    -0.084023    -0.522783      14.15
 O       4.797624    -0.943232     0.127286     244.62
 C       5.407207    -0.500484     1.417204     111.31
 H       4.684809    -0.405608     2.317687      26.06
 H       5.738651     0.661753     1.391489      27.31
 H       6.329962    -1.027599     1.506411      27.89
 C       3.611077    -0.417216    -1.833113      33.50
 O       3.976807    -1.695848    -2.330356     134.25
 H       5.024951    -1.807956    -2.135452      23.30
 C       2.871730     0.481923    -2.708574      99.18
 H       2.896015     0.062677    -3.830148      29.70
 C       2.496639     2.066195    -1.047614      16.81
 C       1.749594     3.308720    -0.364151     108.35
 H       2.066774     4.102945    -1.106620      21.53
 O       2.105132     3.562608     1.101464     308.74
 H       3.036484     3.847111     1.428960      30.28
 C       0.320470     3.555552    -0.662876      54.44
 H       0.098609     3.351237    -1.694081      17.74
 C      -0.236921     4.876311    -0.120541     103.84
 O       0.066789     5.973746    -0.977274     315.54
 H      -0.145336     5.666311    -1.933723      28.99
 H      -0.070477     4.995549     0.957845      25.19
 H      -1.284588     4.833898    -0.296170      21.99
 C      -1.079062    -0.961180    -0.186747      45.88
 H      -0.560201    -1.993918    -0.202091      19.09
 C      -2.846226     0.210796    -1.084446      43.02
 H      -3.729304     0.080046    -1.783442      18.95
 C      -2.295769     1.481506    -0.683364       0.50
 O      -2.864302     2.846045    -0.754036     183.59
 C      -4.042469     3.131184    -1.499703     110.30
 H      -5.007077     2.587216    -1.496986      24.51
 H      -4.507846     4.051929    -1.343172      25.75
 H      -3.751926     3.144818    -2.862781      21.22
 C      -1.017567     1.421413     0.027412      -1.11
 O      -0.371105     2.512189     0.423324     108.65
 C      -0.324698     0.169028     0.140516      31.29
 H       0.483008     0.338978     0.870686      16.33
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 C      -2.209370    -1.083992    -0.916733      29.22
 C      -2.967381    -2.401456    -1.109173      88.27
 H      -3.906932    -2.198281    -1.491075      24.24
 O      -2.140395    -3.284169    -1.896286     278.55
 H      -2.514384    -4.098227    -2.069722      23.15
 C      -3.267412    -3.092639     0.262334      53.60
 H      -2.161200    -3.180452     0.801425      19.05
 O      -4.255237    -2.201562     1.047217     311.76
 H      -4.159595    -2.233340     1.964886      28.42
 C      -4.414618    -4.428316    -0.112737      72.09
 O      -4.076755    -5.283399    -1.288601     263.36
 H      -3.505686    -6.125415    -0.991635      25.75
 H      -5.445521    -3.896157    -0.446409      25.83
 H      -4.298241    -4.787348     0.930101      25.32
55
name = lig-etoh-frame_891
 C       2.324338     1.815163    -2.381510      37.72
 H       1.805788     2.385612    -3.290376      10.25
 C       3.308882     1.186392    -0.207957      55.66
 H       3.299914     1.387120     0.968236      12.88
 C       3.995514    -0.043926    -0.501540      41.43
 O       4.778245    -0.920878     0.176989     280.21
 C       5.406266    -0.486102     1.353475     136.90
 H       4.703302    -0.724503     2.145607      28.15
 H       5.701592     0.490489     1.509432      31.68
 H       6.377307    -1.038232     1.544937      28.02
 C       3.669716    -0.414294    -1.846776      38.35
 O       3.950961    -1.710442    -2.353389     127.65
 H       4.977368    -1.931335    -2.103639      22.58
 C       2.902025     0.501325    -2.695167      48.66
 H       2.797569     0.265186    -3.676923      31.49
 C       2.454977     2.099093    -1.022638     113.80
 C       1.743934     3.393871    -0.418894     125.88
 H       2.197151     4.239044    -1.211254      23.13
 O       2.082064     3.529444     1.087074     289.58
 H       2.926145     4.055917     1.114307      31.39
 C       0.356839     3.532721    -0.637737      58.01
 H      -0.060250     3.497522    -1.686707      14.93
 C      -0.277170     4.810214    -0.156623      96.99
 O       0.093105     5.994399    -0.955914     250.25
 H      -0.020956     5.700369    -1.998592      28.21
 H      -0.130939     5.113555     0.891572      24.94
 H      -1.418586     4.908628    -0.267385      20.43
 C      -1.061890    -0.984167    -0.190109      43.42
 H      -0.606348    -1.984939     0.029818      18.38
 C      -2.846416     0.167745    -1.122082      56.41
 H      -3.696077     0.172099    -1.779171      17.51
 C      -2.252758     1.413924    -0.711754       4.33
 O      -2.873140     2.871807    -0.737630     160.83
 C      -4.022095     3.122366    -1.511017     100.88
 H      -4.907550     2.436051    -1.276026      23.08
 H      -4.492839     4.080730    -0.847800      20.91
 H      -3.692663     2.957345    -2.615795      20.74
 C      -1.054306     1.470288    -0.056190       6.08
 O      -0.356327     2.502326     0.441169     141.21
 C      -0.386106     0.143359     0.154939      12.26
 H       0.739857     0.097558     0.557039      14.02
 C      -2.255430    -1.050899    -0.936879      33.89
 C      -2.957790    -2.397669    -1.133953      82.32
 H      -4.104799    -2.258397    -1.465083      20.56
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 O      -2.137329    -3.296812    -1.852277     253.24
 H      -2.298591    -4.237353    -2.333323      19.23
 C      -3.365500    -3.024227     0.226205      83.58
 H      -2.511791    -3.450918     0.624245      24.22
 O      -4.228142    -2.249201     1.007743     321.20
 H      -3.792672    -2.291896     2.001096      23.82
 C      -4.420230    -4.444597    -0.125652      99.66
 O      -4.070978    -5.285791    -1.226778     333.65
 H      -3.314253    -5.885481    -0.979634      27.47
 H      -5.380236    -4.120447    -0.280629      28.65
 H      -4.577930    -5.024929     0.818013      27.21
55
name = lig-etoh-frame_892
 C       2.321402     1.726077    -2.393611      -7.02
 H       1.877464     2.326600    -3.071221      16.54
 C       3.384942     1.176717    -0.210569      64.76
 H       3.510293     1.432148     0.767505      19.10
 C       4.008694     0.040840    -0.564807      37.62
 O       4.767770    -0.893401     0.211389     243.12
 C       5.417761    -0.493109     1.348183     126.77
 H       4.794321    -0.972521     2.180282      25.90
 H       5.604570     0.681099     1.398599      27.65
 H       6.277337    -1.153494     1.472582      27.09
 C       3.698976    -0.400569    -1.896876      38.54
 O       3.954118    -1.708895    -2.360088     214.81
 H       4.727857    -2.067431    -2.060236      26.10
 C       2.943703     0.525870    -2.679411      20.80
 H       2.716483     0.254975    -3.805836      22.11
 C       2.433163     2.120213    -0.955840      92.97
 C       1.858690     3.452011    -0.451927     106.18
 H       2.344130     4.386473    -0.968898      20.84
 O       2.048186     3.510033     1.021727     331.92
 H       2.833277     4.141802     0.798324      26.69
 C       0.284010     3.504179    -0.571154      87.18
 H      -0.107871     3.183687    -1.534483      18.41
 C      -0.369631     4.819682    -0.185605      90.50
 O       0.135927     6.019415    -0.944743     317.10
 H       0.217907     5.771236    -1.842253      34.21
 H       0.004753     5.122876     0.809744      24.42
 H      -1.418229     4.556918    -0.179289      23.14
 C      -1.014415    -1.076927    -0.192784      16.85
 H      -0.549721    -1.963150     0.245317      20.48
 C      -2.881499     0.185458    -1.198085      64.33
 H      -3.842397     0.366295    -1.724506      21.86
 C      -2.267449     1.410157    -0.747451      -1.12
 O      -2.848934     2.833352    -0.709445     152.49
 C      -4.053772     3.106962    -1.440213     105.12
 H      -4.604458     2.205302    -1.174814      23.78
 H      -4.202808     4.006016    -1.068115      25.92
 H      -3.803172     3.089559    -2.746401      21.50
 C      -1.020214     1.426717    -0.131763      -0.75
 O      -0.333460     2.528655     0.438909     176.70
 C      -0.441607     0.168328     0.167939      38.56
 H       0.575832    -0.039863     0.259363      18.85
 C      -2.296979    -1.031648    -0.926330      18.76
 C      -3.026647    -2.386906    -1.143866      92.79
 H      -3.857404    -2.233648    -1.776462      22.62
 O      -2.078641    -3.311637    -1.840231     229.99
 H      -2.685892    -4.076462    -2.245794      18.33
 C      -3.506860    -3.051182     0.152404      96.30
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 H      -2.700180    -3.727699     0.742256      18.81
 O      -4.186319    -2.282527     1.005105     331.36
 H      -3.615914    -2.247207     1.889135      24.72
 C      -4.391380    -4.438820    -0.106085      99.82
 O      -4.058048    -5.293873    -1.178557     338.88
 H      -3.203793    -5.683396    -0.843326      27.49
 H      -5.521641    -4.053294    -0.295609      24.34
 H      -4.643560    -5.205617     0.673996      25.53
55
name = lig-etoh-frame_893
 C       2.343843     1.649294    -2.286079     100.06
 H       1.789386     2.374352    -3.061473      24.92
 C       3.398066     1.275286    -0.173445      65.73
 H       3.720394     1.667941     0.888959      20.50
 C       4.023714     0.065985    -0.679024      30.27
 O       4.733158    -0.859098     0.182883     237.14
 C       5.430887    -0.498478     1.406382     118.15
 H       4.944100    -0.757175     2.365808      25.93
 H       5.518602     0.530916     1.375207      28.23
 H       6.389045    -1.084296     1.298134      25.24
 C       3.719875    -0.386162    -1.948316      22.18
 O       3.947084    -1.682199    -2.376327     118.70
 H       4.718600    -2.254235    -1.769351      21.82
 C       2.983222     0.500207    -2.747675      41.66
 H       2.798221     0.134409    -3.716004      17.80
 C       2.474450     2.085290    -0.946396      80.33
 C       1.938650     3.450138    -0.457722     102.90
 H       2.420029     4.512452    -0.717631      18.50
 O       2.032866     3.521351     0.919469     344.33
 H       2.855925     4.028718     1.252420      27.17
 C       0.201704     3.461849    -0.519770      77.84
 H      -0.049732     2.891818    -1.451959      16.47
 C      -0.427109     4.867797    -0.198076      82.90
 O       0.162149     6.035739    -0.913427     285.83
 H       0.437873     5.717412    -1.952194      24.51
 H      -0.006650     4.993169     0.812185      23.30
 H      -1.497823     4.490551    -0.182156      21.68
 C      -1.028478    -1.136041    -0.211450      35.26
 H      -0.508868    -2.051115     0.318992      18.96
 C      -2.929457     0.271701    -1.276213      49.89
 H      -3.978538     0.348622    -1.629658      21.97
 C      -2.309449     1.472617    -0.780684      -5.72
 O      -2.786990     2.742589    -0.686298     167.74
 C      -4.049632     3.042010    -1.381035      97.70
 H      -4.762747     2.174568    -1.185436      23.62
 H      -4.325680     4.277244    -1.304139      21.82
 H      -3.996790     3.249766    -2.676530      22.05
 C      -0.947816     1.364489    -0.177267      -5.02
 O      -0.314197     2.552050     0.417922     175.86
 C      -0.489385     0.153262     0.146475      43.86
 H       0.729295     0.112541     0.311422      16.39
 C      -2.304678    -1.072600    -0.872219      -5.80
 C      -3.077268    -2.371604    -1.171851      68.90
 H      -3.722277    -2.163039    -2.153568      18.42
 O      -2.036114    -3.326170    -1.839789     220.55
 H      -2.850811    -3.839680    -2.009322      19.44
 C      -3.604592    -3.221839     0.085064      92.83
 H      -2.735151    -3.498868     0.603308      21.12
 O      -4.163805    -2.272073     1.044230     394.68
 H      -3.733354    -2.170112     1.818105      31.81
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 C      -4.457118    -4.401283    -0.087152     109.21
 O      -4.024215    -5.300728    -1.161206     364.63
 H      -3.124825    -5.741966    -0.805727      24.29
 H      -5.366815    -4.016590    -0.400347      25.50
 H      -4.419411    -5.021210     0.841639      26.20
55
name = lig-etoh-frame_894
 C       2.355177     1.610314    -2.200240     104.62
 H       1.798095     2.141651    -2.872513      29.44
 C       3.416869     1.389616    -0.117065      67.44
 H       3.803674     1.790136     0.785315      25.24
 C       4.034331     0.110555    -0.708908      18.91
 O       4.682263    -0.833869     0.131963     218.99
 C       5.446368    -0.506093     1.445859     105.41
 H       4.958357    -0.630344     2.434088      25.19
 H       5.656915     0.657425     1.462001      25.46
 H       6.483252    -0.829829     1.260166      25.69
 C       3.737480    -0.384993    -1.996013      20.27
 O       3.965248    -1.672142    -2.390009     219.76
 H       4.434529    -2.039929    -1.630707      25.59
 C       3.008512     0.456191    -2.835440      42.95
 H       2.832431     0.104147    -3.868976      18.53
 C       2.570413     2.049419    -0.948344      14.25
 C       1.952564     3.434237    -0.447878      90.01
 H       2.411999     4.381754    -0.963784      16.16
 O       2.040126     3.546795     0.891354     415.65
 H       2.757738     3.690732     1.496530      30.23
 C       0.181707     3.427909    -0.545787      76.11
 H       0.009086     3.044994    -1.570667      18.61
 C      -0.434390     4.885142    -0.203524      86.85
 O       0.177576     6.030156    -0.896320     324.51
 H       0.325675     5.695552    -1.755171      32.21
 H      -0.240069     4.943779     0.894124      23.52
 H      -1.555707     4.980579    -0.310396      23.17
 C      -1.086586    -1.154432    -0.219838      60.16
 H      -0.665984    -2.040346     0.075577      20.39
 C      -2.944167     0.334597    -1.299823      43.25
 H      -3.971981     0.212022    -1.587038      22.98
 C      -2.302228     1.490911    -0.801048       3.43
 O      -2.757950     2.680860    -0.689738     188.98
 C      -4.043585     3.016589    -1.347068     126.61
 H      -4.976426     2.498597    -1.162349      26.81
 H      -4.455699     3.913035    -1.096404      27.70
 H      -4.004785     3.041028    -2.516528      25.37
 C      -0.931291     1.360378    -0.212583     -12.85
 O      -0.317281     2.527542     0.410892     196.07
 C      -0.431523     0.073424     0.112116      47.32
 H       0.460484     0.279398     0.579024      18.83
 C      -2.329180    -1.092685    -0.816318     -14.33
 C      -3.090270    -2.349252    -1.238210      68.98
 H      -3.714128    -2.120966    -2.048876      21.07
 O      -2.017380    -3.327961    -1.836880     110.65
 H      -2.802076    -4.171525    -1.970329      13.55
 C      -3.624423    -3.304615     0.055525      63.19
 H      -2.489325    -3.428474     0.342885      16.69
 O      -4.185491    -2.251957     1.054479     303.40
 H      -3.695747    -2.248616     2.077316      21.14
 C      -4.541621    -4.405319    -0.076647      83.85
 O      -3.976624    -5.302848    -1.151868     349.86
 H      -3.278554    -5.906069    -0.880556      27.77
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 H      -5.602754    -4.054521    -0.453560      24.22
 H      -4.426124    -4.689443     1.002091      25.73
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name = lig-etoh-frame_895
 C       2.382159     1.524255    -2.225097      70.57
 H       1.603922     2.127854    -2.861443      23.59
 C       3.507788     1.403847    -0.092468      48.56
 H       3.861870     1.863116     0.859597      23.42
 C       4.026475     0.202713    -0.651055      23.27
 O       4.648056    -0.819134     0.110139     213.29
 C       5.465131    -0.434089     1.423328     104.54
 H       4.870542    -0.837642     2.310494      24.71
 H       5.668203     0.600620     1.496565      26.58
 H       6.473570    -0.864220     1.382483      26.15
 C       3.739570    -0.366100    -2.031893      20.82
 O       3.995187    -1.666875    -2.396467     177.40
 H       4.357458    -2.028712    -1.534840      23.20
 C       3.001049     0.448066    -2.889955      33.13
 H       2.787821     0.317402    -4.007647      15.22
 C       2.643495     2.090228    -0.921878      53.88
 C       1.923828     3.404546    -0.457957      88.65
 H       2.277290     4.040406    -1.389157      15.96
 O       2.020555     3.579268     0.938445     354.08
 H       3.030079     3.440808     1.318458      22.96
 C       0.220017     3.447521    -0.622339      56.13
 H      -0.062266     3.311299    -1.681426      16.90
 C      -0.431610     4.893631    -0.198929      90.99
 O       0.192682     6.014599    -0.856347     263.89
 H       0.206671     5.697642    -1.885654      26.92
 H      -0.443627     5.033177     0.893316      24.34
 H      -1.452100     5.252144    -0.498491      21.55
 C      -1.144255    -1.132768    -0.215040      31.56
 H      -0.727764    -2.273083    -0.158499      16.30
 C      -2.911640     0.298078    -1.254052      49.64
 H      -3.977831     0.247182    -1.625149      24.38
 C      -2.229845     1.411169    -0.814472      14.04
 O      -2.798155     2.702771    -0.709368     159.37
 C      -4.049435     2.979137    -1.306811      88.79
 H      -5.014046     2.421323    -0.977147      23.81
 H      -4.340163     4.044366    -0.656602      21.45
 H      -3.839196     2.822693    -2.642693      20.62
 C      -0.952437     1.338252    -0.230729      -6.76
 O      -0.343210     2.457359     0.396435     152.27
 C      -0.370744     0.036592     0.062029      16.77
 H       0.409971     0.127142     1.021765      15.84
 C      -2.401822    -1.044038    -0.817606       2.22
 C      -3.066628    -2.362592    -1.283143      71.33
 H      -3.970050    -2.087779    -2.001484      19.89
 O      -2.047040    -3.343861    -1.838780     200.41
 H      -2.276201    -4.208844    -1.936722      21.73
 C      -3.561089    -3.200142     0.043846      69.02
 H      -2.621931    -3.756133     0.216386      18.53
 O      -4.198068    -2.247785     1.062546     316.41
 H      -3.924634    -2.564902     1.933864      25.20
 C      -4.617725    -4.436555    -0.081101      91.03
 O      -3.959495    -5.294151    -1.147083     345.61
 H      -3.394389    -6.117459    -0.728787      26.49
 H      -5.657143    -4.262304    -0.344309      26.98
 H      -4.789032    -4.756476     0.981844      28.13
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name = lig-etoh-frame_896
 C       2.381385     1.507522    -2.277711      38.27
 H       1.577335     2.029649    -2.770949      23.82
 C       3.628056     1.396396    -0.085179      55.75
 H       3.881009     1.739428     0.964386      20.38
 C       4.023621     0.235253    -0.611517      26.78
 O       4.649451    -0.795265     0.127833     231.54
 C       5.458865    -0.382098     1.360842     115.34
 H       4.878892    -0.892284     2.090139      27.36
 H       5.544501     0.751053     1.489563      26.72
 H       6.358279    -1.070846     1.424789      25.95
 C       3.736387    -0.315048    -2.024059      26.89
 O       4.041903    -1.657013    -2.384866     134.34
 H       4.413235    -2.226580    -1.494354      20.86
 C       2.978276     0.467153    -2.923312      15.07
 H       2.778409     0.398724    -3.929011      18.76
 C       2.666482     2.126642    -0.928695      90.87
 C       1.833531     3.334312    -0.503012     107.53
 H       2.181375     4.103943    -1.317770      15.33
 O       2.031138     3.622062     0.995571     317.48
 H       2.965061     3.554235     0.863291      28.13
 C       0.275823     3.502168    -0.669004      42.20
 H      -0.182550     3.352539    -1.690232      18.27
 C      -0.432816     4.907943    -0.197762      88.79
 O       0.242778     5.999201    -0.833033     274.43
 H       0.085813     5.945326    -1.857548      28.74
 H      -0.446785     5.110430     0.883343      24.55
 H      -1.491007     4.839008    -0.645357      21.71
 C      -1.173648    -1.129891    -0.216592      16.06
 H      -0.827231    -2.064064    -0.205119      19.44
 C      -2.897682     0.185534    -1.179671      81.64
 H      -3.812138     0.452233    -1.661359      23.51
 C      -2.172397     1.362406    -0.825783       3.13
 O      -2.828475     2.714343    -0.723607     168.57
 C      -4.091236     2.975002    -1.251380     129.38
 H      -4.712830     2.168454    -0.894142      24.63
 H      -4.039071     3.909819    -0.912672      25.78
 H      -3.966990     2.927010    -2.334872      24.85
 C      -0.935053     1.273613    -0.210112       5.84
 O      -0.374938     2.384621     0.342518     131.04
 C      -0.334112     0.030185     0.060862      32.54
 H       0.257113    -0.208480     0.829451      20.11
 C      -2.464255    -0.987169    -0.877270      31.40
 C      -3.070117    -2.415274    -1.292286      89.43
 H      -3.969578    -2.269475    -1.855777      23.91
 O      -2.069451    -3.302072    -1.857372     166.19
 H      -2.128526    -4.409519    -1.775966      16.19
 C      -3.557247    -3.076016     0.040380      74.09
 H      -2.774300    -3.868149     0.449746      18.04
 O      -4.188985    -2.268732     1.035541     275.56
 H      -4.116309    -2.730596     1.952709      24.44
 C      -4.645919    -4.448768    -0.101636      90.87
 O      -3.974194    -5.296323    -1.125168     337.98
 H      -3.551618    -6.004309    -0.627707      30.52
 H      -5.728066    -4.258836    -0.487395      26.78
 H      -4.895806    -5.076669     0.806387      28.30
55
name = lig-etoh-frame_897
 C       2.357050     1.600438    -2.260518      33.67
 H       1.536102     2.049467    -2.866067      22.70
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 C       3.684145     1.458083    -0.098466     109.79
 H       3.865020     1.585385     0.932554      18.32
 C       4.046796     0.153461    -0.639611      31.80
 O       4.680147    -0.759826     0.157653     263.71
 C       5.425787    -0.373159     1.278528     123.23
 H       4.768188    -0.698977     2.211436      26.46
 H       5.527546     0.713575     1.453913      30.43
 H       6.313078    -0.960871     1.250084      27.77
 C       3.745050    -0.280233    -1.977125      26.25
 O       4.096902    -1.637417    -2.350225     221.18
 H       4.472829    -2.115522    -1.711184      27.77
 C       2.979238     0.475918    -2.905295      33.10
 H       2.769222     0.201721    -4.044297      22.40
 C       2.668686     2.093451    -0.978997      76.22
 C       1.719205     3.293795    -0.540731     115.91
 H       2.140078     4.357310    -0.786096      16.50
 O       2.050836     3.659824     0.992554     154.58
 H       3.052861     3.964373     0.877523      29.26
 C       0.293744     3.527918    -0.671634      47.19
 H      -0.107958     3.235952    -1.616978      22.86
 C      -0.427436     4.888618    -0.229487      97.88
 O       0.295222     6.007958    -0.814270     296.15
 H       0.117701     6.035137    -1.732446      32.31
 H      -0.380226     5.076387     0.853837      26.29
 H      -1.396191     4.426693    -0.522964      23.00
 C      -1.208141    -1.082632    -0.250000      31.58
 H      -0.735913    -2.176867    -0.036697      18.30
 C      -2.942069     0.209035    -1.136226      43.77
 H      -3.821886     0.480101    -1.778776      20.66
 C      -2.171014     1.354738    -0.831029      -0.91
 O      -2.776703     2.671842    -0.724316     142.97
 C      -4.118529     2.942837    -1.181886      82.88
 H      -4.763193     2.066774    -0.780053      21.74
 H      -4.311263     4.209540    -1.085153      20.90
 H      -4.239076     3.044604    -2.639099      19.72
 C      -0.893042     1.224603    -0.175232      18.17
 O      -0.383862     2.353510     0.277477     146.07
 C      -0.377612    -0.041225     0.057252      40.13
 H       0.610318    -0.366702     0.712628      18.14
 C      -2.436066    -1.092114    -0.930374      37.55
 C      -3.089607    -2.468629    -1.234663      93.48
 H      -3.985918    -2.448624    -1.988065      22.35
 O      -2.071644    -3.257513    -1.895062     221.09
 H      -2.443668    -4.092735    -1.482883      20.14
 C      -3.614095    -3.072174     0.086434      85.97
 H      -2.784705    -3.486915     0.703742      20.96
 O      -4.168472    -2.269372     0.997710     258.09
 H      -4.301237    -2.724915     1.975963      24.76
 C      -4.666622    -4.442285    -0.167183      89.60
 O      -4.024757    -5.288454    -1.106064     337.46
 H      -3.463414    -5.977714    -0.637515      26.95
 H      -5.567960    -4.045360    -0.692583      26.12
 H      -4.728630    -5.167398     0.661029      26.79
55
name = lig-etoh-frame_898
 C       2.336819     1.691613    -2.275184      37.22
 H       1.557573     2.185174    -2.944963      20.56
 C       3.677606     1.484238    -0.193551      83.17
 H       3.771069     1.664598     0.964031      17.03
 C       4.064437     0.118787    -0.664715      28.37
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 O       4.711908    -0.748953     0.157487     276.14
 C       5.369452    -0.372001     1.260452     132.18
 H       4.892914    -0.480123     2.193948      29.08
 H       5.663246     0.713757     1.272616      30.14
 H       6.442427    -0.787749     1.157192      27.02
 C       3.764218    -0.303785    -1.945009      14.30
 O       4.136217    -1.581348    -2.339439     186.82
 H       4.753290    -2.042865    -1.592222      22.34
 C       2.984249     0.492761    -2.845592      45.62
 H       2.827706     0.049242    -3.748165      25.56
 C       2.641603     2.075706    -1.004181      66.50
 C       1.717961     3.330877    -0.492101     123.38
 H       2.095232     4.324073    -0.728619      20.47
 O       2.081420     3.679254     0.960146     213.02
 H       2.818203     4.341038     1.170540      30.88
 C       0.263018     3.489560    -0.652783      70.52
 H       0.007483     3.147757    -1.724490      21.04
 C      -0.378592     4.822852    -0.259515      94.26
 O       0.323743     6.023304    -0.781450     245.80
 H       0.213602     5.992719    -1.895551      25.46
 H      -0.290936     4.932193     0.827742      25.31
 H      -1.516246     4.591772    -0.425962      22.86
 C      -1.220062    -1.147135    -0.291715      58.60
 H      -0.810426    -2.007295     0.120260      22.34
 C      -3.009649     0.270506    -1.142431      23.88
 H      -3.893606     0.281184    -1.756902      19.38
 C      -2.203973     1.344320    -0.808230      11.98
 O      -2.708583     2.629091    -0.738668     188.61
 C      -4.130525     2.937034    -1.193135     136.62
 H      -4.915530     2.378467    -0.741109      27.65
 H      -4.632063     3.804614    -0.942540      28.26
 H      -4.408318     2.876033    -2.075063      30.90
 C      -0.887102     1.199683    -0.174083       0.74
 O      -0.353893     2.377537     0.241713     151.54
 C      -0.392612    -0.122750     0.091453      67.61
 H       0.628823    -0.152422     0.252996      22.63
 C      -2.404312    -1.196581    -0.972885      11.95
 C      -3.134993    -2.461991    -1.183858      97.55
 H      -3.873150    -2.432276    -1.988273      22.44
 O      -2.089939    -3.233650    -1.904058     221.67
 H      -2.491222    -4.060697    -1.582752      19.99
 C      -3.667097    -3.193383     0.154823      68.87
 H      -2.555967    -3.392643     0.659430      20.65
 O      -4.198563    -2.205778     0.991054     337.68
 H      -4.265900    -2.571888     1.797888      31.31
 C      -4.634072    -4.397612    -0.238029      90.87
 O      -4.071051    -5.297151    -1.125453     377.81
 H      -3.266355    -5.887390    -0.775412      25.75
 H      -5.521571    -3.896142    -0.694324      26.00
 H      -4.829617    -4.866405     0.776195      26.13
55
name = lig-etoh-frame_899
 C       2.336863     1.718073    -2.362118      39.98
 H       1.671669     2.305385    -2.921452      18.83
 C       3.625371     1.444714    -0.296594      72.49
 H       3.677639     1.864805     0.640893      18.97
 C       4.067157     0.186575    -0.648951      29.43
 O       4.721820    -0.783388     0.114559     245.82
 C       5.406513    -0.310612     1.285298     122.60
 H       4.911130    -0.483850     2.337780      26.31
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 H       5.693367     0.749660     1.011024      29.62
 H       6.369242    -0.784775     1.332041      28.00
 C       3.770380    -0.333400    -1.943821      20.30
 O       4.180977    -1.542834    -2.329074     166.70
 H       4.997046    -1.764119    -1.660822      21.79
 C       2.987326     0.527445    -2.723369      53.36
 H       2.765397    -0.016456    -3.737562      24.30
 C       2.586353     2.128996    -0.979334      64.07
 C       1.837297     3.422536    -0.383541     110.18
 H       2.150341     4.224547    -1.307950      20.78
 O       2.072285     3.674390     0.950486     315.63
 H       2.635222     4.420920     1.090046      30.69
 C       0.218382     3.379397    -0.663343      94.96
 H       0.080953     3.214421    -1.694090      21.53
 C      -0.337479     4.763706    -0.264264      94.22
 O       0.325168     6.023060    -0.777350     273.46
 H       0.414387     5.866178    -1.690511      32.60
 H      -0.164933     4.785757     0.826550      24.23
 H      -1.407242     5.048465    -0.478062      23.53
 C      -1.201241    -1.280203    -0.310337      23.64
 H      -0.836483    -2.280200     0.158348      20.48
 C      -3.036180     0.214876    -1.174521      54.73
 H      -4.046423     0.227342    -1.637541      22.76
 C      -2.257403     1.318895    -0.760226      12.21
 O      -2.682363     2.630308    -0.771192     135.13
 C      -4.135351     2.894101    -1.138556      79.70
 H      -4.936205     2.298417    -0.507759      23.95
 H      -4.519006     3.973149    -0.577463      22.00
 H      -4.395545     2.542553    -2.491333      20.59
 C      -0.920989     1.171376    -0.203534     -11.30
 O      -0.304837     2.417874     0.234873     160.95
 C      -0.413560    -0.094530     0.092287      45.12
 H       0.755725    -0.106639     0.070934      20.11
 C      -2.427875    -1.150644    -0.990912       9.32
 C      -3.175749    -2.441305    -1.161043      67.66
 H      -4.044640    -2.236179    -1.875013      21.89
 O      -2.122825    -3.240956    -1.881518     140.07
 H      -2.282026    -4.347454    -2.097623      16.99
 C      -3.646786    -3.301062     0.189700      82.37
 H      -2.669977    -3.655950     0.431086      24.86
 O      -4.255511    -2.126001     0.975960     275.20
 H      -4.206604    -2.437699     2.017037      23.93
 C      -4.580660    -4.321840    -0.232453      99.56
 O      -4.094697    -5.330764    -1.178801     360.31
 H      -3.325259    -5.727220    -0.815158      33.42
 H      -5.536095    -3.852628    -0.675775      25.52
 H      -5.127205    -4.557696     0.731461      26.76
55
name = lig-etoh-frame_900
 C       2.357676     1.737950    -2.377720      57.44
 H       1.717042     2.378818    -3.144919      17.91
 C       3.520720     1.432862    -0.355518      57.92
 H       3.817586     2.012637     0.616912      16.98
 C       4.073011     0.220365    -0.654801      32.71
 O       4.733369    -0.822258     0.083009     223.38
 C       5.476692    -0.226785     1.317677     120.59
 H       4.860965    -0.384649     2.152619      28.81
 H       5.630157     0.802630     1.092143      31.45
 H       6.347057    -0.953008     1.512960      26.05
 C       3.758396    -0.295100    -1.909776      24.79
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 O       4.251039    -1.529571    -2.326744     211.92
 H       5.000808    -1.652883    -1.861659      28.06
 C       2.964801     0.522965    -2.677809      63.88
 H       2.697795     0.217246    -3.663614      26.53
 C       2.528177     2.198335    -0.996871      71.76
 C       1.952508     3.496565    -0.394408     103.32
 H       2.226383     4.095144    -1.233193      23.06
 O       2.041775     3.670169     0.960224     327.30
 H       2.693938     4.444784     0.973130      26.58
 C       0.230903     3.299332    -0.682708      75.17
 H       0.034304     3.110886    -1.801182      20.34
 C      -0.307808     4.748369    -0.243470      87.45
 O       0.337415     6.002028    -0.760390     233.20
 H       0.569287     5.792173    -1.763880      27.51
 H      -0.121392     4.735257     0.839766      24.33
 H      -1.323751     5.189638    -0.525320      22.06
 C      -1.152510    -1.369879    -0.297327      17.10
 H      -0.917270    -2.447653    -0.099470      17.74
 C      -3.024915     0.105593    -1.203736      82.71
 H      -4.059763     0.295740    -1.449209      25.38
 C      -2.317631     1.285823    -0.710271      -2.48
 O      -2.705703     2.649818    -0.813605     157.07
 C      -4.171680     2.840540    -1.084273     135.51
 H      -4.583093     2.082547    -0.471277      26.48
 H      -3.957090     3.828043    -0.838412      25.46
 H      -4.152218     2.660986    -1.975126      29.77
 C      -0.979965     1.173594    -0.235656       0.63
 O      -0.275192     2.410313     0.243507     160.88
 C      -0.419759    -0.072881     0.038687      33.89
 H       0.646874    -0.205484     0.248449      20.01
 C      -2.457007    -1.069767    -0.954175       5.47
 C      -3.213219    -2.451699    -1.171305      63.35
 H      -4.213521    -2.172415    -1.600214      20.93
 O      -2.153576    -3.283035    -1.871192     248.05
 H      -2.349464    -3.988014    -2.397214      23.39
 C      -3.589371    -3.270845     0.159211      70.90
 H      -2.662762    -3.966904     0.610358      19.09
 O      -4.303525    -2.104503     0.978647     282.27
 H      -4.058963    -2.100037     1.989748      25.58
 C      -4.616794    -4.266842    -0.210397     100.10
 O      -4.127952    -5.352177    -1.218456     294.81
 H      -3.306824    -5.800588    -0.721512      26.57
 H      -5.369690    -3.787640    -0.827490      26.73
 H      -5.208728    -4.715167     0.602095      26.99
55
name = lig-etoh-frame_901
 C       2.359635     1.793498    -2.344713      35.61
 H       1.918312     2.171829    -3.179921      19.89
 C       3.416403     1.486386    -0.298570      89.55
 H       3.927761     1.835788     0.544047      20.92
 C       4.079756     0.188064    -0.669306      33.79
 O       4.768942    -0.813662     0.089111     215.18
 C       5.529696    -0.192655     1.318477     105.25
 H       4.630809    -0.193451     2.080458      23.60
 H       5.782667     0.949127     1.286750      28.39
 H       6.317869    -0.891601     1.565740      26.21
 C       3.750981    -0.259665    -1.883991      22.59
 O       4.297370    -1.510910    -2.348164     120.03
 H       5.280556    -1.713737    -1.844208      22.93
 C       2.909114     0.519749    -2.716800      60.69
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 H       2.701312     0.266775    -3.764588      25.44
 C       2.507458     2.239159    -1.062334      47.59
 C       1.964792     3.467637    -0.499923     138.38
 H       2.453010     4.617218    -0.945395      20.53
 O       2.028642     3.697942     0.977176     280.71
 H       2.853045     4.261104     1.164518      29.83
 C       0.293337     3.316740    -0.728987      62.46
 H      -0.018708     2.921638    -1.670857      21.83
 C      -0.290544     4.763047    -0.229099      89.83
 O       0.381873     5.964656    -0.750038     260.14
 H       0.565112     5.850683    -1.782172      26.94
 H      -0.181151     4.786709     0.865619      24.19
 H      -1.402242     4.752315    -0.429459      23.91
 C      -1.133436    -1.329901    -0.305132      47.66
 H      -0.819794    -2.375087    -0.297129      18.27
 C      -3.012582     0.102575    -1.200632      71.64
 H      -4.079876     0.205275    -1.408696      27.46
 C      -2.355259     1.279953    -0.686849       0.46
 O      -2.721774     2.623556    -0.849754     150.91
 C      -4.124272     2.795503    -0.979279      87.80
 H      -4.630348     1.974345    -0.304535      22.33
 H      -4.080843     4.002735    -1.009296      21.34
 H      -4.288756     2.669641    -2.405399      20.18
 C      -1.028284     1.195743    -0.245078      -2.16
 O      -0.275323     2.339359     0.258671     145.37
 C      -0.429438    -0.141380    -0.038201      32.50
 H       0.543325    -0.190597     0.540932      20.11
 C      -2.437230    -1.144022    -0.864589      -3.27
 C      -3.210784    -2.464393    -1.157966      81.02
 H      -4.183641    -2.373292    -1.598075      20.65
 O      -2.191609    -3.296889    -1.869447     231.49
 H      -2.780896    -3.834009    -2.630143      19.73
 C      -3.515340    -3.179329     0.138103     103.02
 H      -2.935383    -3.726680     0.835081      21.62
 O      -4.324952    -2.118078     0.977513     352.34
 H      -3.908343    -2.036678     1.815653      30.68
 C      -4.705225    -4.263011    -0.233772      70.15
 O      -4.150772    -5.354969    -1.219182     287.16
 H      -3.484889    -5.947824    -0.775765      26.81
 H      -5.304370    -3.650242    -1.014087      24.44
 H      -5.113220    -4.948565     0.548259      25.07
55
name = lig-etoh-frame_902
 C       2.366132     1.778091    -2.359376      47.40
 H       1.838572     2.311642    -3.269776      20.82
 C       3.380110     1.477642    -0.201186      77.93
 H       3.815572     1.882514     0.757095      23.16
 C       4.047279     0.194295    -0.631115      12.38
 O       4.835609    -0.744734     0.120510     221.47
 C       5.505966    -0.157582     1.318750     121.89
 H       4.741877    -0.069194     2.025587      27.09
 H       6.010277     0.773426     1.234905      29.70
 H       6.349572    -0.818938     1.615564      26.71
 C       3.745632    -0.279630    -1.944025      12.31
 O       4.344376    -1.478898    -2.375183     181.03
 H       5.160715    -1.701197    -1.865692      25.69
 C       2.856394     0.530458    -2.772330      53.43
 H       2.799732     0.142397    -3.847908      24.38
 C       2.561008     2.263550    -1.088588      43.11
 C       1.913288     3.501688    -0.580662     124.95
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 H       2.329355     4.497680    -0.739807      19.42
 O       2.027773     3.720035     0.979703     300.38
 H       2.948997     3.887267     1.242144      30.27
 C       0.377059     3.395051    -0.733374      35.37
 H      -0.002264     2.922263    -1.687469      20.72
 C      -0.290554     4.760759    -0.236489     100.63
 O       0.424248     5.917875    -0.745856     285.85
 H       0.389651     5.886016    -1.684646      30.79
 H      -0.174234     4.846410     0.858460      24.59
 H      -1.340076     4.335450    -0.378909      22.18
 C      -1.148623    -1.253998    -0.339338      58.69
 H      -0.486856    -2.240373    -0.331438      19.40
 C      -3.003374     0.127394    -1.143241      44.88
 H      -4.024473     0.031535    -1.522617      25.83
 C      -2.352022     1.290995    -0.702675      18.73
 O      -2.734115     2.572146    -0.873461     251.81
 C      -4.068901     2.791209    -0.987709     151.18
 H      -4.790777     2.338076    -0.340400      28.13
 H      -4.675105     3.705226    -0.850608      26.58
 H      -4.552810     2.568623    -1.824861      29.56
 C      -1.017724     1.174374    -0.221488      -3.22
 O      -0.283532     2.247148     0.268313     100.83
 C      -0.428248    -0.175853    -0.094750      42.46
 H       0.365446    -0.103612     0.703433      20.67
 C      -2.434574    -1.248920    -0.794654       7.44
 C      -3.130975    -2.469930    -1.113459      83.12
 H      -4.050675    -2.500076    -1.861568      18.29
 O      -2.256826    -3.325205    -1.908041     263.79
 H      -3.059602    -3.609160    -2.526373      20.27
 C      -3.572568    -3.098073     0.169084      89.09
 H      -2.750828    -3.428538     0.953370      20.07
 O      -4.333689    -2.153159     0.950304     335.75
 H      -3.661730    -2.093985     1.827225      23.76
 C      -4.732904    -4.285948    -0.309864      83.23
 O      -4.183075    -5.341192    -1.213090     333.34
 H      -3.622030    -5.982768    -0.759224      28.68
 H      -5.502193    -3.751280    -0.818486      27.94
 H      -5.134984    -4.789546     0.565894      25.81
55
name = lig-etoh-frame_903
 C       2.354497     1.744253    -2.446947      51.57
 H       1.789736     2.462048    -2.962611      22.20
 C       3.405049     1.422513    -0.106886      47.00
 H       3.418231     1.910439     0.887971      20.23
 C       3.974044     0.230172    -0.588327       3.07
 O       4.909589    -0.635410     0.151598     203.77
 C       5.483543    -0.135381     1.309333     111.55
 H       4.796809     0.051464     2.238469      25.19
 H       6.158715     0.757976     0.935633      25.58
 H       6.226832    -0.920705     1.693916      25.49
 C       3.736660    -0.287929    -1.999513      11.66
 O       4.368063    -1.436832    -2.421257     197.03
 H       5.057586    -1.642280    -1.773584      24.93
 C       2.861599     0.494511    -2.828066      57.24
 H       2.796953     0.127429    -3.787857      24.22
 C       2.664568     2.263718    -1.065230      45.77
 C       1.841749     3.514257    -0.564128      94.26
 H       2.279057     4.661647    -1.088566      15.69
 O       2.023735     3.723562     0.966952     336.35
 H       3.033663     3.543279     1.071314      26.20
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 C       0.437489     3.472749    -0.711625      39.23
 H       0.134142     3.222313    -1.731984      20.51
 C      -0.284498     4.697812    -0.232868     103.77
 O       0.441709     5.870178    -0.741934     203.94
 H       0.156365     5.944258    -1.807537      25.29
 H      -0.116366     4.816459     0.834617      25.19
 H      -1.342158     4.597036    -0.516000      24.31
 C      -1.131063    -1.277140    -0.383459      35.64
 H      -0.497958    -2.065238    -0.229955      23.03
 C      -2.994975     0.073633    -1.045040      59.77
 H      -3.904286     0.056599    -1.656733      24.69
 C      -2.304380     1.266785    -0.737424      13.63
 O      -2.742477     2.557113    -0.892817     193.43
 C      -4.135032     2.810695    -0.987931     111.73
 H      -4.725252     2.324079    -0.040375      24.47
 H      -4.610426     3.800694    -0.664485      24.01
 H      -4.831677     2.129621    -1.892651      21.71
 C      -0.973539     1.116013    -0.197518      13.47
 O      -0.276026     2.177500     0.277395      73.67
 C      -0.411810    -0.069919    -0.091529      40.45
 H       0.429405    -0.173312     0.551779      21.59
 C      -2.458575    -1.222503    -0.782428      24.26
 C      -3.070176    -2.490769    -1.102066      95.94
 H      -3.857476    -2.170212    -1.738192      23.13
 O      -2.327091    -3.364027    -1.965434     328.08
 H      -2.895508    -3.796092    -2.482864      27.38
 C      -3.692168    -3.097612     0.223732      91.49
 H      -2.631053    -3.275549     0.558511      23.12
 O      -4.325949    -2.179434     0.943281     372.15
 H      -3.916767    -2.091574     1.802209      29.03
 C      -4.694976    -4.319114    -0.355026      87.51
 O      -4.233588    -5.310778    -1.211688     319.42
 H      -3.638860    -5.945131    -0.598520      25.44
 H      -5.740934    -3.866221    -0.671249      25.27
 H      -5.171942    -4.564728     0.664547      25.23
55
name = lig-etoh-frame_904
 C       2.373735     1.741152    -2.438657      47.67
 H       1.677758     2.476872    -2.956439      21.94
 C       3.403387     1.404590    -0.060789      85.32
 H       3.220536     1.627445     0.984625      22.03
 C       3.921896     0.226054    -0.574242       8.80
 O       4.934973    -0.530784     0.141240     210.32
 C       5.512483    -0.091946     1.331636     125.59
 H       4.899730     0.271807     2.129117      28.37
 H       6.088110     0.705598     0.994973      27.47
 H       6.023682    -0.978387     1.680265      27.14
 C       3.721789    -0.243624    -1.982151      15.64
 O       4.384411    -1.389315    -2.477664     135.47
 H       4.972954    -1.671073    -1.546902      20.01
 C       2.902264     0.445182    -2.875044      50.76
 H       2.674363     0.074630    -3.971751      23.51
 C       2.741024     2.221075    -1.062053      57.51
 C       1.872661     3.516564    -0.487924      94.98
 H       2.122535     4.459984    -1.301199      16.97
 O       2.033746     3.711118     0.917596     325.99
 H       3.005103     3.556187     0.963913      28.77
 C       0.410423     3.500693    -0.710559      37.14
 H       0.209604     3.426654    -1.787906      20.45
 C      -0.281459     4.655020    -0.210831     105.78
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 O       0.430083     5.836759    -0.766305     208.00
 H       0.183606     5.958598    -1.669436      30.40
 H      -0.195637     4.706665     0.895865      25.29
 H      -1.280084     5.029237    -0.603452      23.12
 C      -1.075678    -1.264765    -0.405866      40.09
 H      -0.587030    -2.352228    -0.085878      24.50
 C      -3.007360     0.025421    -0.958874      60.03
 H      -3.836243     0.194324    -1.649232      22.39
 C      -2.247526     1.207636    -0.769170      -0.20
 O      -2.756623     2.568997    -0.922199     132.95
 C      -4.313959     2.765196    -0.943491     122.01
 H      -4.368938     2.222940    -0.019307      24.88
 H      -4.040860     3.924862    -0.934706      22.91
 H      -4.584843     2.279644    -1.738495      26.49
 C      -0.964988     1.148364    -0.204905      28.84
 O      -0.239171     2.166822     0.289997      21.91
 C      -0.375767    -0.061597    -0.057642      37.10
 H       0.748924    -0.225970     0.225093      24.07
 C      -2.408707    -1.167096    -0.788250      24.32
 C      -3.110285    -2.488326    -1.135444      75.70
 H      -3.997279    -1.851141    -1.619556      22.23
 O      -2.357978    -3.398426    -2.012507     219.15
 H      -2.877840    -4.246563    -2.504697      17.95
 C      -3.748091    -3.173432     0.158342      86.04
 H      -2.757841    -3.615340     0.535674      23.21
 O      -4.357294    -2.170530     0.966162     332.39
 H      -4.152184    -2.159643     1.949430      27.79
 C      -4.703886    -4.293338    -0.295746     110.46
 O      -4.269965    -5.303925    -1.194555     337.39
 H      -3.648914    -5.815151    -0.698743      31.42
 H      -5.543754    -3.903498    -0.791312      27.70
 H      -5.008103    -4.738729     0.654654      27.26
55
name = lig-etoh-frame_905
 C       2.433100     1.742821    -2.363060      53.61
 H       1.737023     2.190598    -3.083807      22.31
 C       3.363813     1.407799    -0.073157     107.60
 H       3.235702     1.329182     1.050819      20.76
 C       3.919696     0.189918    -0.581389      28.43
 O       4.907539    -0.458407     0.082840     201.67
 C       5.554754    -0.029636     1.360948      97.16
 H       4.770507     0.465907     2.035978      26.34
 H       6.359220     0.843493     1.247669      24.50
 H       5.989525    -1.041732     1.757454      25.53
 C       3.721427    -0.201842    -1.941498      20.74
 O       4.408769    -1.336288    -2.483870     215.99
 H       4.800359    -1.757763    -1.798660      28.37
 C       2.916302     0.459096    -2.917068      48.97
 H       2.668822     0.064587    -3.829912      26.50
 C       2.737697     2.178018    -1.063693      58.96
 C       1.938184     3.476432    -0.431593     118.90
 H       2.127587     4.215976    -1.292651      21.10
 O       2.066785     3.698013     0.852411     315.08
 H       3.031189     3.893879     1.126264      28.99
 C       0.343572     3.442829    -0.730012      35.84
 H       0.153412     3.321864    -1.839941      20.55
 C      -0.311272     4.708120    -0.174707     103.69
 O       0.434463     5.827940    -0.762629     256.74
 H       0.247170     5.868835    -1.780572      26.98
 H      -0.337159     4.673655     0.912444      25.21
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 H      -1.323083     4.884678    -0.500428      24.70
 C      -0.984342    -1.266061    -0.376636      70.32
 H      -0.811494    -2.220500    -0.187579      26.37
 C      -3.023787     0.059626    -0.917280      44.43
 H      -3.961333     0.187303    -1.487423      21.95
 C      -2.232580     1.202363    -0.784445      13.42
 O      -2.752775     2.548382    -0.964411     105.90
 C      -4.375855     2.754071    -0.864447      97.89
 H      -4.516759     2.181476     0.154597      22.40
 H      -4.115431     3.690424    -1.193592      24.24
 H      -4.705231     2.351195    -2.057097      21.46
 C      -0.949602     1.209351    -0.224036     -10.89
 O      -0.180034     2.224216     0.289998      67.61
 C      -0.286959    -0.165805    -0.034246      41.40
 H       0.750472    -0.081752    -0.058801      25.93
 C      -2.311901    -1.207726    -0.802047      14.88
 C      -3.224585    -2.441839    -1.183313      83.67
 H      -4.077799    -2.164914    -1.678547      26.02
 O      -2.382007    -3.423179    -2.065796     208.91
 H      -2.908727    -4.307248    -2.068096      19.05
 C      -3.718379    -3.259065     0.051400      93.45
 H      -3.163175    -3.981630     0.765095      20.33
 O      -4.398097    -2.152471     0.991643     215.12
 H      -4.308269    -2.523848     2.034600      24.67
 C      -4.752384    -4.260132    -0.194125      90.02
 O      -4.284240    -5.312665    -1.182139     282.48
 H      -3.509209    -5.853220    -0.823657      28.40
 H      -5.535844    -3.754029    -0.888613      25.46
 H      -4.983383    -4.981216     0.644481      27.31
55
name = lig-etoh-frame_906
 C       2.500798     1.701026    -2.337923      63.86
 H       1.835824     2.163821    -3.051682      22.70
 C       3.324045     1.351270    -0.114467      54.71
 H       3.315125     1.482762     0.937103      20.65
 C       3.926677     0.204600    -0.606869      24.09
 O       4.911438    -0.427462     0.042617     204.05
 C       5.577478     0.047489     1.380722     113.87
 H       4.741875     0.453816     1.940811      28.01
 H       6.436851     0.616613     1.322761      28.13
 H       5.911372    -0.818662     1.828493      29.35
 C       3.739063    -0.203854    -1.944162      35.13
 O       4.419998    -1.273569    -2.487486     186.22
 H       4.854628    -1.969812    -1.824627      23.82
 C       2.937506     0.536669    -2.849106      55.94
 H       2.686172     0.044988    -3.846092      24.87
 C       2.656055     2.176978    -1.011288      66.82
 C       1.955537     3.373487    -0.499385     132.16
 H       2.418589     4.421032    -1.226570      17.89
 O       2.129522     3.699021     0.847864     292.90
 H       2.874338     4.329623     1.150294      29.32
 C       0.296305     3.346496    -0.707747      61.63
 H       0.002306     3.021853    -1.694536      22.23
 C      -0.352724     4.773433    -0.168344      89.37
 O       0.435780     5.842968    -0.744219     269.58
 H       0.425389     5.638865    -1.799025      24.99
 H      -0.294586     4.801824     0.947587      24.21
 H      -1.486550     4.532571    -0.404754      22.51
 C      -0.944786    -1.312770    -0.347091      31.47
 H      -0.560645    -2.486072    -0.267654      21.24
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 C      -2.996054     0.070836    -0.914790      37.09
 H      -4.057490     0.060094    -1.166208      21.49
 C      -2.247394     1.274619    -0.771007      12.72
 O      -2.761091     2.503253    -1.005881     149.86
 C      -4.343193     2.696523    -0.870156      99.17
 H      -4.967731     2.407997    -0.040149      26.10
 H      -4.626149     3.922871    -1.041548      23.70
 H      -4.906743     2.323276    -1.595355      27.20
 C      -0.874739     1.174370    -0.225938     -34.06
 O      -0.126284     2.313862     0.254522     130.30
 C      -0.208580    -0.160170    -0.042069      45.57
 H       0.936055    -0.020298    -0.065082      23.68
 C      -2.307972    -1.234843    -0.839476       8.46
 C      -3.259522    -2.446126    -1.203735      70.65
 H      -4.224171    -2.397448    -1.921904      20.81
 O      -2.421101    -3.421570    -2.089121     213.87
 H      -2.968323    -4.213955    -1.799853      19.50
 C      -3.691329    -3.310603     0.038882      99.38
 H      -3.060089    -3.816627     0.742016      23.34
 O      -4.422501    -2.177482     1.017647     246.48
 H      -4.375623    -2.656057     1.760398      27.77
 C      -4.843485    -4.274619    -0.164576     100.21
 O      -4.280062    -5.328036    -1.178723     284.91
 H      -3.445595    -5.862777    -0.842995      27.44
 H      -5.700891    -3.793177    -0.592627      28.73
 H      -5.210507    -4.816166     0.708236      29.79
55
name = lig-etoh-frame_907
 C       2.508255     1.726822    -2.337128      44.64
 H       1.891437     2.445060    -2.960867      21.46
 C       3.274563     1.299046    -0.142767      69.71
 H       3.445011     1.847042     0.851739      21.69
 C       3.949054     0.240944    -0.650732      28.37
 O       4.976209    -0.436264     0.049377     195.96
 C       5.538240     0.094894     1.357681     104.20
 H       4.791939     0.593761     1.999741      23.64
 H       6.535616     0.660846     1.068334      24.31
 H       5.811030    -0.906671     1.977050      24.48
 C       3.769026    -0.231320    -1.957990      37.35
 O       4.441169    -1.235326    -2.500915     197.81
 H       4.864413    -1.964867    -1.809975      22.04
 C       2.996070     0.551649    -2.756508      65.22
 H       2.778458     0.239710    -3.790076      24.26
 C       2.561439     2.148859    -0.960775      85.87
 C       1.939390     3.365324    -0.629747     137.44
 H       2.470627     4.185945    -0.865757      23.40
 O       2.172745     3.696800     0.877905     321.64
 H       2.768834     4.466224     0.835228      32.42
 C       0.294376     3.281959    -0.645945      72.02
 H      -0.156898     2.850563    -1.616097      19.72
 C      -0.381360     4.772440    -0.183312      94.36
 O       0.412278     5.856033    -0.737067     325.31
 H       0.547801     5.673672    -1.635421      32.49
 H      -0.137714     4.947120     0.865708      25.00
 H      -1.407972     4.581923    -0.392671      24.91
 C      -0.941244    -1.419806    -0.340464       2.49
 H      -0.280698    -2.198813    -0.375998      18.97
 C      -2.920223     0.045176    -0.924632      51.92
 H      -4.026554    -0.000417    -0.849949      22.99
 C      -2.234770     1.302251    -0.717388      -2.80
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 O      -2.831502     2.492283    -1.036002     182.88
 C      -4.297782     2.709003    -0.892161     117.79
 H      -5.050271     2.533900     0.015314      24.17
 H      -4.711001     3.620439    -0.754781      26.31
 H      -5.057977     1.981834    -1.613376      22.75
 C      -0.791159     1.114510    -0.225294      -6.64
 O      -0.102009     2.369708     0.215835     161.62
 C      -0.148371    -0.081271    -0.085781      25.70
 H       0.885668    -0.172498     0.182336      21.29
 C      -2.355540    -1.226818    -0.869310      -2.91
 C      -3.239251    -2.505258    -1.228937      80.68
 H      -4.073142    -2.229302    -1.821167      23.24
 O      -2.470369    -3.398385    -2.086135     213.01
 H      -2.967957    -4.369126    -1.787402      16.22
 C      -3.729125    -3.288384     0.096217      78.21
 H      -2.586384    -3.480598     0.514431      19.83
 O      -4.424257    -2.231116     0.999026     251.76
 H      -4.419220    -2.750340     1.937483      24.43
 C      -4.909941    -4.327302    -0.168897      81.71
 O      -4.278612    -5.341199    -1.169711     308.16
 H      -3.628889    -5.786696    -0.665532      32.16
 H      -5.908354    -3.864349    -0.504663      26.75
 H      -5.324203    -4.638993     0.852077      28.18
55
name = lig-etoh-frame_908
 C       2.453154     1.839015    -2.311027      34.31
 H       2.036029     2.537560    -2.985292      21.79
 C       3.227813     1.311591    -0.106003      81.26
 H       3.622481     1.902504     0.691806      24.13
 C       4.025298     0.238431    -0.658364      19.55
 O       5.046433    -0.454002     0.078299     220.95
 C       5.501523     0.095580     1.317584     139.39
 H       4.937810     0.875739     1.915020      23.84
 H       6.305441     0.662135     0.933696      27.00
 H       5.710508    -0.716521     1.877353      28.45
 C       3.805114    -0.250026    -1.933225      28.39
 O       4.490841    -1.254850    -2.530375     257.89
 H       4.832950    -1.689352    -1.850116      29.10
 C       3.041162     0.553176    -2.734585      48.57
 H       2.955940     0.357313    -3.769329      24.38
 C       2.484614     2.056250    -0.993868      56.73
 C       1.862103     3.404505    -0.643227     101.45
 H       2.508395     4.395995    -1.209469      19.55
 O       2.186873     3.678497     0.890520     342.27
 H       2.774845     4.427265     0.686466      29.75
 C       0.313229     3.314791    -0.660170      88.96
 H      -0.075888     3.119234    -1.633015      20.96
 C      -0.337317     4.724721    -0.205321      84.16
 O       0.369641     5.876751    -0.724137     262.78
 H       0.584624     5.804060    -1.810537      25.97
 H      -0.147031     4.866547     0.885650      23.28
 H      -1.478442     4.895721    -0.489524      22.25
 C      -0.957475    -1.400101    -0.370446       0.02
 H      -0.112225    -2.234517    -0.483299      17.55
 C      -2.853770     0.043112    -0.913968      52.85
 H      -3.924146     0.086058    -0.772446      24.06
 C      -2.186190     1.239346    -0.649854     -11.65
 O      -2.922442     2.512152    -1.041155     154.37
 C      -4.326908     2.650439    -0.902456     109.92
 H      -4.445287     2.235463     0.147113      24.39
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 H      -4.455298     3.914838    -0.951208      22.86
 H      -4.650169     2.099680    -1.676977      25.70
 C      -0.756237     1.152622    -0.240451       5.77
 O      -0.117756     2.330676     0.246243     186.34
 C      -0.148120    -0.100786    -0.140091       1.62
 H       0.800595    -0.252861     0.442460      20.95
 C      -2.329233    -1.279510    -0.863010       1.43
 C      -3.206717    -2.538445    -1.228073      78.26
 H      -4.109070    -1.920977    -1.750761      21.19
 O      -2.523056    -3.401266    -2.061719     296.52
 H      -2.817250    -4.239948    -2.078332      26.86
 C      -3.774901    -3.196136     0.157027      92.17
 H      -2.783101    -3.448039     0.341881      24.77
 O      -4.405926    -2.323425     0.974316     330.96
 H      -4.407237    -2.446364     2.024224      25.42
 C      -4.927168    -4.374071    -0.164481      83.07
 O      -4.301722    -5.346351    -1.131214     311.75
 H      -3.769272    -5.875751    -0.415630      27.46
 H      -5.773743    -3.928066    -0.724931      26.43
 H      -5.151247    -4.779320     0.835749      27.38
55
name = lig-etoh-frame_909
 C       2.416011     1.857127    -2.351681      42.56
 H       2.098491     2.578923    -3.162032      20.81
 C       3.246669     1.303010    -0.075152      81.30
 H       3.660054     1.829814     0.798279      23.06
 C       4.106196     0.235278    -0.587789      12.68
 O       5.072545    -0.475254     0.085791     236.88
 C       5.475968     0.131648     1.267910     125.51
 H       4.860120     0.902285     1.662314      24.07
 H       6.459320     0.731733     1.006147      25.54
 H       5.808688    -0.744811     2.035508      24.78
 C       3.831317    -0.240596    -1.921842       5.53
 O       4.546379    -1.294670    -2.569109     166.63
 H       5.108794    -1.711977    -1.707352      21.27
 C       3.038437     0.628206    -2.759291      35.74
 H       3.205279     0.343909    -3.896833      22.52
 C       2.394396     2.034116    -1.004631      42.62
 C       1.821473     3.475347    -0.571536      91.20
 H       1.972370     4.008599    -1.457710      23.15
 O       2.180500     3.661851     0.847075     327.29
 H       2.936786     4.358347     0.938178      27.67
 C       0.320870     3.430244    -0.706657      55.52
 H       0.040008     3.331609    -1.819903      17.84
 C      -0.291511     4.688019    -0.226950     106.63
 O       0.346701     5.910348    -0.733261     295.00
 H       0.302252     5.878961    -1.685951      31.97
 H      -0.299003     4.640378     0.867256      24.10
 H      -1.278833     4.951491    -0.490009      23.45
 C      -0.926646    -1.309577    -0.437936      76.70
 H      -0.481227    -2.294037    -0.484395      20.59
 C      -2.816380     0.023076    -0.875455      30.31
 H      -3.918184     0.187850    -1.002447      23.84
 C      -2.137638     1.193068    -0.612287      -2.82
 O      -2.915569     2.516617    -1.030289     128.84
 C      -4.330335     2.626785    -0.869073     112.63
 H      -4.215732     1.979282     0.038240      22.06
 H      -4.322411     3.576693    -1.149762      25.54
 H      -4.767781     2.108231    -1.956214      22.97
 C      -0.767302     1.224321    -0.265572     -13.76
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 O      -0.145360     2.253615     0.301003     122.33
 C      -0.200064    -0.183753    -0.171910       5.70
 H       0.681115    -0.201511     0.483660      22.25
 C      -2.237859    -1.355984    -0.831876       7.33
 C      -3.234274    -2.485383    -1.194013      86.13
 H      -4.010039    -1.944588    -1.712028      22.12
 O      -2.540964    -3.393273    -2.049500     232.27
 H      -2.982852    -4.374190    -2.294686      19.39
 C      -3.826933    -3.158364     0.139917      79.00
 H      -2.923245    -3.871547     0.671874      19.54
 O      -4.410616    -2.355247     0.989265     372.47
 H      -4.171676    -2.312929     1.871438      31.00
 C      -4.867589    -4.388545    -0.182187      91.46
 O      -4.325183    -5.365131    -1.051634     288.48
 H      -3.857349    -6.096514    -0.510915      27.76
 H      -5.668094    -3.952001    -0.795408      25.92
 H      -5.100745    -5.012854     0.722761      25.87
55
name = lig-etoh-frame_910
 C       2.400147     1.800486    -2.439735      49.28
 H       2.067241     2.516820    -3.164386      21.51
 C       3.302342     1.289193    -0.086447      67.50
 H       3.370132     1.724378     0.949898      19.06
 C       4.122613     0.236430    -0.545333      12.68
 O       5.079146    -0.507431     0.078610     246.06
 C       5.533390     0.171269     1.257486     132.42
 H       4.629085     0.783825     1.553752      24.14
 H       6.485906     0.626500     1.156290      28.73
 H       5.709961    -0.496009     2.026264      29.05
 C       3.851142    -0.194921    -1.936241      -0.58
 O       4.597988    -1.328146    -2.560585     164.30
 H       5.357785    -1.718073    -1.987734      23.65
 C       3.069679     0.680924    -2.823138      45.15
 H       3.273956     0.442797    -3.785630      24.70
 C       2.334985     2.079150    -0.953560      37.13
 C       1.785277     3.449837    -0.476414      73.28
 H       1.921189     4.135231    -1.550019      17.22
 O       2.176226     3.680551     0.776978     343.75
 H       2.978559     4.067945     1.155490      28.95
 C       0.320606     3.520941    -0.750122      48.58
 H       0.117011     3.208422    -1.743565      18.76
 C      -0.282555     4.707492    -0.220039      96.66
 O       0.339270     5.950632    -0.716712     249.23
 H       0.081966     5.890942    -1.747772      27.17
 H      -0.307597     4.590352     0.881628      22.78
 H      -1.409160     4.648664    -0.556905      20.71
 C      -0.885537    -1.297807    -0.522788      74.48
 H      -0.592344    -2.385742    -0.336539      24.24
 C      -2.811463    -0.046717    -0.836174      32.51
 H      -3.758229     0.111479    -1.359213      23.57
 C      -2.135304     1.207755    -0.627849       3.68
 O      -2.802629     2.490406    -1.013482     156.34
 C      -4.297420     2.514559    -0.897981     104.22
 H      -4.838871     2.053769     0.028678      24.85
 H      -4.611045     3.777454    -1.000147      23.34
 H      -4.977899     2.177064    -1.589683      26.49
 C      -0.797750     1.192750    -0.282475       2.88
 O      -0.158527     2.218865     0.333867      32.18
 C      -0.248497    -0.157989    -0.165755      41.56
 H       0.713395    -0.222051     0.313678      23.08
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 C      -2.224110    -1.333848    -0.809776       6.59
 C      -3.241204    -2.436305    -1.120944      77.31
 H      -4.104062    -2.000295    -1.785048      20.71
 O      -2.538770    -3.407024    -2.058949     236.92
 H      -3.284396    -4.079518    -2.177635      21.26
 C      -3.814244    -3.271376     0.096472     107.81
 H      -3.245251    -3.842973     0.720453      22.30
 O      -4.463777    -2.314747     1.037619     318.26
 H      -3.734937    -2.275930     1.891502      24.30
 C      -4.788507    -4.377824    -0.203123     104.18
 O      -4.326826    -5.423358    -1.000332     339.52
 H      -3.874799    -6.135465    -0.653242      32.22
 H      -5.780637    -3.973140    -0.647380      25.79
 H      -5.258825    -4.865123     0.693166      26.02
55
name = lig-etoh-frame_911
 C       2.376108     1.761253    -2.428398      57.90
 H       1.925940     2.458059    -3.164762      21.22
 C       3.304858     1.328585    -0.114687      97.67
 H       3.088958     1.528825     0.918921      15.16
 C       4.082738     0.219961    -0.599353      12.21
 O       5.093952    -0.543193     0.077378     229.21
 C       5.567565     0.200758     1.271480     116.46
 H       4.759517     0.796515     1.640455      26.95
 H       6.537739     0.718748     1.018278      26.40
 H       5.592842    -0.603567     2.154593      26.17
 C       3.901650    -0.146225    -1.952202      18.19
 O       4.626089    -1.325972    -2.543970     180.11
 H       5.406627    -1.602768    -2.125690      25.45
 C       3.159551     0.661083    -2.869184      37.16
 H       3.269293     0.501675    -4.049793      22.02
 C       2.363118     2.090229    -0.954572      69.35
 C       1.785365     3.389282    -0.503779     115.20
 H       2.284571     4.248088    -0.949347      20.22
 O       2.151880     3.725609     0.763095     311.97
 H       3.132711     3.858884     0.977190      30.21
 C       0.348232     3.522235    -0.741887      38.73
 H       0.053408     2.999671    -1.703576      19.07
 C      -0.362450     4.774236    -0.199046     100.20
 O       0.315172     5.982468    -0.692610     269.35
 H       0.127088     5.967028    -1.733336      28.12
 H      -0.187722     4.785187     0.881145      24.46
 H      -1.348374     4.453507    -0.489738      23.40
 C      -0.856543    -1.386794    -0.588265      34.51
 H      -0.307477    -2.289251    -0.137056      24.01
 C      -2.831578    -0.057962    -0.837435      61.39
 H      -3.673032    -0.079882    -1.547561      22.50
 C      -2.192382     1.217401    -0.690093      12.56
 O      -2.703431     2.430686    -0.978614     155.68
 C      -4.290852     2.472259    -0.889041     106.13
 H      -5.040203     2.321851    -0.081313      24.90
 H      -4.613258     3.382447    -0.681947      26.82
 H      -5.004022     1.949025    -1.735089      23.32
 C      -0.824959     1.118152    -0.262069      17.08
 O      -0.168900     2.222147     0.338665      49.55
 C      -0.248801    -0.077581    -0.144812      20.34
 H       0.855928    -0.213579     0.068145      19.34
 C      -2.288267    -1.262855    -0.799690      19.96
 C      -3.207140    -2.436980    -1.063870      74.58
 H      -4.118421    -2.075555    -1.646258      22.42
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 O      -2.553891    -3.409399    -2.057009     242.66
 H      -3.307959    -3.946620    -2.136747      24.51
 C      -3.808835    -3.349318     0.079964      77.37
 H      -2.862938    -3.798616     0.786775      19.71
 O      -4.498394    -2.274698     1.097899     296.70
 H      -3.741061    -2.189407     1.689505      25.68
 C      -4.804505    -4.372636    -0.203548     104.07
 O      -4.324110    -5.493464    -1.007855     301.55
 H      -3.686160    -6.166443    -0.474658      26.11
 H      -5.704227    -3.997281    -0.632979      27.70
 H      -5.221605    -4.536937     0.825656      25.76
55
name = lig-etoh-frame_912
 C       2.373017     1.726242    -2.356909      83.29
 H       1.762940     2.300067    -3.077714      23.85
 C       3.262698     1.372085    -0.159348     126.68
 H       3.022274     1.345042     0.955618      16.12
 C       4.036771     0.203373    -0.668091      10.22
 O       5.089084    -0.552666     0.083132     230.33
 C       5.586285     0.183694     1.305332     118.44
 H       4.976117     1.041961     1.718344      26.85
 H       6.451382     0.758667     0.911080      25.32
 H       5.726927    -0.606305     2.010559      28.56
 C       3.996030    -0.139243    -2.012749      23.43
 O       4.611802    -1.285163    -2.530490     138.08
 H       5.586398    -1.422894    -1.972373      19.87
 C       3.246193     0.639451    -2.926409      42.84
 H       3.233214     0.500839    -3.942081      22.78
 C       2.462210     2.045464    -1.037578      38.40
 C       1.848034     3.358962    -0.573105     130.53
 H       2.548942     4.239988    -0.888198      16.99
 O       2.124281     3.771234     0.835116     317.24
 H       3.094371     3.783619     0.629483      25.54
 C       0.351670     3.451536    -0.692540      51.59
 H      -0.060684     3.091733    -1.625497      19.79
 C      -0.414050     4.817986    -0.178278      85.64
 O       0.263761     6.013398    -0.677566     281.01
 H       0.317251     6.006585    -1.626448      32.56
 H      -0.163420     4.972104     0.891675      23.53
 H      -1.542148     4.718052    -0.393004      22.68
 C      -0.838296    -1.416482    -0.578835      47.63
 H      -0.173537    -2.194758    -0.240258      25.42
 C      -2.907393     0.031226    -0.904037      60.29
 H      -3.840282    -0.108453    -1.460833      21.79
 C      -2.218339     1.160948    -0.742992      20.65
 O      -2.687176     2.382419    -0.928059     158.66
 C      -4.320583     2.424435    -0.895494      76.70
 H      -4.632470     1.931461     0.134171      23.20
 H      -4.393283     3.719958    -0.805740      21.68
 H      -4.421222     1.957688    -1.865475      22.66
 C      -0.873010     1.122763    -0.213475       2.55
 O      -0.186245     2.246820     0.315950     101.33
 C      -0.201857    -0.129853    -0.164499      17.58
 H       0.850776    -0.034645    -0.061639      19.41
 C      -2.280057    -1.288461    -0.771310      -2.54
 C      -3.176321    -2.489515    -1.038071      80.95
 H      -4.124398    -2.037595    -1.478357      22.29
 O      -2.567299    -3.384792    -2.035466     195.75
 H      -3.305827    -4.203128    -2.288917      17.03
 C      -3.729461    -3.323799     0.138336      86.00
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 H      -2.846448    -3.661141     0.482878      23.40
 O      -4.515107    -2.269837     1.116736     299.13
 H      -3.839184    -2.035254     1.769175      26.27
 C      -4.860562    -4.397041    -0.179367      73.37
 O      -4.318505    -5.578864    -1.006967     290.19
 H      -3.601776    -5.844349    -0.365619      28.16
 H      -5.661951    -3.923125    -0.902194      24.97
 H      -5.096260    -4.519006     0.918551      24.20
55
name = lig-etoh-frame_913
 C       2.418269     1.635380    -2.373616      54.27
 H       1.662879     2.140016    -2.941976      23.06
 C       3.264434     1.308114    -0.178497      74.90
 H       3.157151     1.419435     0.856839      18.05
 C       4.018878     0.213029    -0.682184       5.38
 O       5.038175    -0.525051     0.091628     215.48
 C       5.599166     0.172988     1.297005     115.31
 H       5.043365     1.023468     1.708650      27.28
 H       6.541003     0.643899     0.937332      25.72
 H       5.991881    -0.631767     2.027225      26.13
 C       4.080181    -0.139515    -2.114951      22.09
 O       4.630200    -1.240349    -2.507088     192.23
 H       5.368249    -1.346754    -1.935416      23.57
 C       3.276483     0.666687    -2.927434      66.21
 H       3.236825     0.379663    -4.056486      20.46
 C       2.546313     2.041618    -1.099471      39.80
 C       1.919722     3.381564    -0.608902      95.73
 H       2.330338     4.049172    -1.440563      17.67
 O       2.103476     3.783180     0.898370     296.93
 H       3.094891     3.984885     0.896626      26.97
 C       0.292124     3.375252    -0.623308      63.38
 H      -0.138200     3.263259    -1.652511      18.91
 C      -0.423646     4.838432    -0.156447      88.16
 O       0.198682     6.051924    -0.660697     234.56
 H       0.509829     5.891428    -1.714743      27.56
 H      -0.311836     4.935466     0.932516      24.44
 H      -1.488069     5.087747    -0.291849      23.16
 C      -0.843531    -1.357721    -0.508761      77.18
 H      -0.225976    -2.404100    -0.583102      20.82
 C      -2.992706     0.007733    -1.002573      21.64
 H      -4.069876     0.084061    -1.209406      19.86
 C      -2.183265     1.128402    -0.755618       2.36
 O      -2.730664     2.381059    -0.871369     184.08
 C      -4.264230     2.435263    -0.874377     114.14
 H      -4.229764     1.602459    -0.176589      22.65
 H      -4.321848     3.372369    -1.103196      26.20
 H      -4.300196     2.014671    -1.936766      23.98
 C      -0.894314     1.117767    -0.165629       2.32
 O      -0.209123     2.283216     0.272325     162.85
 C      -0.170491    -0.195634    -0.223520      23.25
 H       0.918720     0.020834    -0.031120      18.62
 C      -2.229537    -1.335877    -0.746267     -15.37
 C      -3.185425    -2.543126    -1.046445      84.10
 H      -4.133085    -1.955725    -1.416887      19.36
 O      -2.588877    -3.371924    -2.018910     285.45
 H      -2.989576    -4.177413    -2.232729      23.31
 C      -3.684634    -3.228110     0.204920      62.45
 H      -2.659811    -3.860355     0.636460      18.52
 O      -4.497307    -2.308227     1.096442     291.84
 H      -4.029485    -1.871728     2.020769      23.50
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 C      -4.880094    -4.401450    -0.173730      87.71
 O      -4.315482    -5.634584    -0.963234     312.23
 H      -3.505073    -5.790474    -0.483395      29.74
 H      -5.552923    -3.970308    -0.814077      26.98
 H      -5.274028    -4.834864     0.761428      25.39
55
name = lig-etoh-frame_914
 C       2.461557     1.560182    -2.456811      57.42
 H       1.609741     2.023909    -3.020872      23.12
 C       3.305796     1.194302    -0.191224      55.08
 H       3.370115     1.652848     0.868884      21.49
 C       4.059122     0.212536    -0.689910      27.68
 O       4.957454    -0.482141     0.107205     252.36
 C       5.639676     0.148724     1.252146     109.11
 H       4.930240     0.803792     1.732171      24.95
 H       6.637138     0.534378     0.882017      24.61
 H       6.009034    -0.596360     2.027593      25.97
 C       4.098474    -0.061905    -2.138428      21.69
 O       4.685195    -1.240998    -2.513989     176.34
 H       5.364630    -1.534759    -1.789724      21.47
 C       3.290897     0.665936    -2.967730      67.99
 H       3.197711     0.312523    -3.986655      20.71
 C       2.598389     2.079592    -1.079595      63.79
 C       1.923987     3.409862    -0.617355      56.49
 H       1.985539     4.041255    -1.596015      20.68
 O       2.114786     3.778841     0.896579     301.55
 H       2.891898     4.288200     1.367253      26.41
 C       0.203744     3.340104    -0.577383      74.52
 H      -0.093914     3.280508    -1.640224      18.79
 C      -0.408036     4.856775    -0.106572      86.13
 O       0.160365     6.087569    -0.670095     296.63
 H       0.409774     5.788992    -1.514692      34.28
 H      -0.372051     4.802334     0.999296      24.91
 H      -1.495054     4.982405    -0.379945      23.67
 C      -0.858142    -1.349403    -0.446116      58.42
 H      -0.524531    -2.259650    -0.762447      21.12
 C      -2.991124    -0.111507    -1.065793      31.08
 H      -4.059165     0.123582    -0.980711      20.09
 C      -2.174061     1.134410    -0.745974     -18.41
 O      -2.759354     2.412955    -0.811908     176.80
 C      -4.105975     2.381635    -0.922843     101.96
 H      -4.609076     1.533798    -0.214145      22.92
 H      -4.655448     3.590422    -1.004935      21.39
 H      -4.674769     1.994062    -1.895214      23.16
 C      -0.861870     1.059509    -0.156344      15.83
 O      -0.239733     2.310129     0.228944     173.28
 C      -0.138392    -0.149586    -0.264570      30.71
 H       0.915792    -0.228133     0.012272      19.88
 C      -2.253856    -1.334326    -0.765869      -4.80
 C      -3.209138    -2.541948    -1.046369      76.04
 H      -4.093147    -2.082100    -1.510324      20.15
 O      -2.578180    -3.354959    -2.014091     251.86
 H      -2.985042    -4.305175    -2.057900      20.04
 C      -3.664736    -3.199867     0.310995      91.97
 H      -3.015385    -3.727017     0.855302      23.31
 O      -4.454114    -2.350750     1.071632     386.87
 H      -4.204453    -2.138647     1.917994      33.09
 C      -4.820918    -4.424315    -0.156780      78.82
 O      -4.317692    -5.649748    -0.902836     267.61
 H      -3.329680    -5.971577    -0.629343      25.23
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 H      -5.693589    -3.913331    -0.801973      23.61
 H      -5.522653    -5.012016     0.536444      23.34
55
name = lig-etoh-frame_915
 C       2.442647     1.606474    -2.477275      62.58
 H       1.728663     1.944431    -3.185666      25.68
 C       3.311248     1.196418    -0.180194      77.37
 H       3.614734     1.662183     0.728009      24.87
 C       4.147357     0.195315    -0.726793      35.20
 O       4.893543    -0.479327     0.131003     284.95
 C       5.680211     0.111955     1.188426     109.36
 H       4.951535     0.735127     1.818359      23.16
 H       6.523603     0.634218     0.787045      26.54
 H       5.836381    -0.734216     1.906401      25.65
 C       4.127517    -0.015931    -2.072505      13.23
 O       4.769896    -1.250995    -2.539262     191.15
 H       5.175123    -1.801057    -1.662714      20.79
 C       3.315778     0.604186    -3.050813      33.60
 H       3.160925     0.250755    -4.073920      20.83
 C       2.627927     2.087882    -1.063453      40.11
 C       1.866973     3.416753    -0.595335      79.89
 H       1.889732     4.336979    -1.268138      17.82
 O       2.131533     3.762534     0.856757     349.65
 H       2.606937     4.526438     1.296964      29.15
 C       0.166417     3.375080    -0.580218      67.88
 H      -0.103560     3.124333    -1.622575      18.18
 C      -0.415429     4.846921    -0.048909      85.18
 O       0.134133     6.102303    -0.657893     266.22
 H       0.305734     5.802556    -1.661563      27.19
 H      -0.311536     4.833200     1.047211      23.48
 H      -1.423262     4.567616    -0.454501      21.47
 C      -0.924930    -1.337763    -0.418570      14.25
 H      -0.422085    -2.415651    -0.760312      16.95
 C      -2.895082    -0.159668    -1.058811      59.31
 H      -3.989020    -0.165843    -0.995435      22.09
 C      -2.194184     1.104988    -0.725784     -14.28
 O      -2.744741     2.433576    -0.754465     197.47
 C      -4.103235     2.360237    -0.995960     142.12
 H      -4.876468     1.960073    -0.172758      24.09
 H      -4.547167     3.140018    -0.577532      26.41
 H      -4.595224     1.986796    -1.890398      26.08
 C      -0.829115     1.048106    -0.209473      16.20
 O      -0.288152     2.297370     0.224162     169.07
 C      -0.106207    -0.116015    -0.270536      22.59
 H       0.916194    -0.355403    -0.012900      19.47
 C      -2.335601    -1.304949    -0.814466      18.60
 C      -3.205066    -2.513801    -1.007243      54.91
 H      -4.222890    -2.255412    -1.606340      19.63
 O      -2.551296    -3.368866    -2.024173     197.80
 H      -3.043808    -4.300278    -1.731831      17.28
 C      -3.721172    -3.254431     0.372640      69.18
 H      -2.910944    -3.718713     1.223272      19.23
 O      -4.436802    -2.363110     1.039480     307.77
 H      -4.170125    -2.464758     2.080020      22.66
 C      -4.770596    -4.466315    -0.147245      91.43
 O      -4.297716    -5.646242    -0.860855     347.00
 H      -3.482746    -6.055334    -0.584083      30.08
 H      -5.422823    -3.959857    -0.784026      27.35
 H      -5.446454    -4.796559     0.635879      26.40
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name = lig-etoh-frame_916
 C       2.456958     1.664761    -2.473036      68.42
 H       1.743031     2.149135    -3.159240      26.06
 C       3.328117     1.282141    -0.201098      55.61
 H       3.685571     1.607181     0.807661      22.10
 C       4.191501     0.253173    -0.731238      31.69
 O       4.865819    -0.543822     0.159684     282.62
 C       5.668612     0.075963     1.149901     110.04
 H       5.204421     0.778503     1.805620      25.51
 H       6.478521     0.766730     0.710183      25.24
 H       5.921855    -0.937014     1.683094      23.86
 C       4.183700    -0.085016    -2.074639       9.12
 O       4.854813    -1.255827    -2.545959     265.18
 H       4.958066    -1.773284    -1.849774      29.21
 C       3.305815     0.571854    -3.066002      33.97
 H       3.212101     0.161393    -4.150651      19.70
 C       2.606763     2.090351    -1.089788      36.20
 C       1.774673     3.439006    -0.527080     101.16
 H       2.126223     4.444991    -0.981169      15.97
 O       2.135091     3.722130     0.807919     329.49
 H       2.473335     4.626760     0.752138      27.48
 C       0.210747     3.424640    -0.614201      70.38
 H      -0.192042     3.123030    -1.615675      17.99
 C      -0.428545     4.785512    -0.032163      85.38
 O       0.109190     6.073652    -0.644283     246.07
 H       0.040678     6.016498    -1.694955      28.57
 H      -0.269498     4.970736     1.036272      22.50
 H      -1.458024     4.536453    -0.291737      21.51
 C      -0.976007    -1.350711    -0.445650      51.64
 H      -0.391069    -2.174619    -0.363631      21.34
 C      -2.849068    -0.049811    -1.018181      56.11
 H      -3.900550    -0.289383    -1.264005      22.77
 C      -2.187779     1.066163    -0.692723       9.27
 O      -2.713494     2.400210    -0.700772     164.47
 C      -4.209545     2.350902    -1.012678      82.57
 H      -4.695318     1.833224    -0.156400      24.43
 H      -4.396222     3.558523    -0.470506      20.43
 H      -4.301228     2.038799    -2.192665      21.73
 C      -0.826269     1.107996    -0.307731     -14.99
 O      -0.342178     2.264271     0.260574     184.62
 C      -0.119562    -0.181105    -0.260294       7.29
 H       1.008443    -0.232450    -0.052517      18.59
 C      -2.332400    -1.347425    -0.836454       6.28
 C      -3.205485    -2.519700    -0.973431      76.99
 H      -4.155862    -2.264961    -1.369115      25.06
 O      -2.536915    -3.413688    -2.000497     267.88
 H      -2.871346    -4.201208    -1.787730      23.93
 C      -3.731608    -3.400649     0.381426      86.91
 H      -2.892710    -3.622265     0.895386      25.17
 O      -4.451141    -2.322537     1.066948     298.44
 H      -4.394502    -2.708027     2.059254      23.85
 C      -4.703835    -4.500410    -0.107769      73.92
 O      -4.275509    -5.635672    -0.839401     323.22
 H      -3.553173    -6.118746    -0.269775      27.34
 H      -5.259692    -3.922259    -0.959744      25.12
 H      -5.240368    -4.555187     0.924489      26.18
55
name = lig-etoh-frame_917
 C       2.514180     1.692485    -2.483828      29.59
 H       1.812716     2.404487    -2.953070      15.99
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 C       3.399631     1.389052    -0.239335      37.58
 H       3.408186     1.580473     0.872691      17.47
 C       4.189740     0.342111    -0.714616      18.55
 O       4.837384    -0.626549     0.172123     251.25
 C       5.681587     0.031070     1.124208     133.46
 H       5.221884     0.750020     1.902482      26.44
 H       6.468650     0.566897     0.626217      27.87
 H       6.253937    -0.775529     1.594818      27.35
 C       4.201542    -0.184033    -2.154653       5.74
 O       4.928942    -1.237106    -2.564246     223.33
 H       4.914954    -1.973166    -1.745457      22.98
 C       3.279191     0.573449    -2.994623      58.69
 H       3.274948     0.224336    -3.966554      26.33
 C       2.535059     2.116030    -1.131418      38.58
 C       1.699467     3.446256    -0.493966     112.92
 H       2.308208     4.183935    -1.127109      18.44
 O       2.144421     3.683545     0.789512     315.46
 H       2.447421     4.574939     0.463933      24.49
 C       0.260895     3.458255    -0.641473      74.37
 H      -0.180246     3.337200    -1.608488      19.33
 C      -0.437475     4.719444    -0.053799      92.93
 O       0.068174     6.024706    -0.630484     265.47
 H      -0.127610     6.024415    -1.527609      34.31
 H      -0.205361     4.947640     1.010921      23.14
 H      -1.587189     4.812308    -0.036250      22.01
 C      -0.962236    -1.356965    -0.474962      69.02
 H      -0.387113    -2.293415     0.089555      21.86
 C      -2.881162    -0.005270    -0.990551      38.62
 H      -3.826279     0.100181    -1.576359      22.37
 C      -2.155729     1.122840    -0.655347      11.15
 O      -2.716755     2.333091    -0.658972     163.21
 C      -4.265008     2.429209    -0.971714     105.73
 H      -4.611809     1.438119    -0.376586      22.19
 H      -4.348535     3.449589    -1.081454      25.13
 H      -4.357451     2.291948    -1.950628      28.86
 C      -0.793635     1.112362    -0.396172     -10.18
 O      -0.371918     2.250628     0.304104     124.57
 C      -0.187968    -0.217173    -0.255016      33.48
 H       0.836782    -0.152962    -0.079667      20.19
 C      -2.275939    -1.367874    -0.826632      -1.97
 C      -3.195822    -2.595116    -0.943031      67.64
 H      -4.282133    -2.075969    -1.240529      20.98
 O      -2.527623    -3.437907    -1.959250     192.43
 H      -2.795555    -4.512634    -1.909214      16.94
 C      -3.698234    -3.467357     0.308225      74.79
 H      -2.605190    -3.796669     0.760732      20.20
 O      -4.470338    -2.316361     1.115676     269.46
 H      -4.647219    -2.512865     1.994711      28.05
 C      -4.664117    -4.478571    -0.056333     108.97
 O      -4.223132    -5.643545    -0.801048     288.56
 H      -3.760748    -6.214102    -0.062744      27.87
 H      -5.322291    -4.004891    -0.758357      28.41
 H      -5.212552    -4.681894     0.836105      28.51
55
name = lig-etoh-frame_918
 C       2.564189     1.736753    -2.473847      46.92
 H       1.982645     2.383147    -3.143169      16.44
 C       3.459599     1.495783    -0.271430      61.72
 H       3.172382     1.618847     0.753692      16.78
 C       4.193019     0.355027    -0.737709       1.12
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 O       4.793305    -0.681901     0.171692     241.90
 C       5.723688    -0.017750     1.116411     105.34
 H       5.155564     0.498351     1.841191      28.30
 H       6.451192     0.540271     0.414645      25.89
 H       6.554144    -0.647106     1.694262      26.02
 C       4.149364    -0.191579    -2.165454       6.63
 O       4.996218    -1.243358    -2.573834     231.89
 H       5.028969    -1.983142    -1.843768      23.53
 C       3.273970     0.573833    -2.891080      53.93
 H       3.215430     0.352850    -4.067318      25.91
 C       2.471993     2.128726    -1.138835      50.46
 C       1.717172     3.379558    -0.555297     116.71
 H       2.088373     4.027329    -1.438961      21.05
 O       2.158447     3.668993     0.791749     311.53
 H       2.670940     4.544650     0.928783      29.92
 C       0.218657     3.480325    -0.638672      72.47
 H      -0.084589     3.383260    -1.738225      18.68
 C      -0.453202     4.713247    -0.046602     106.83
 O       0.026820     5.965431    -0.599214     247.12
 H      -0.251408     5.919408    -1.653907      28.83
 H      -0.066655     4.676818     0.983844      24.01
 H      -1.502709     4.813168     0.011107      24.25
 C      -0.876592    -1.420793    -0.446621      69.95
 H      -0.688061    -2.250728     0.088208      23.05
 C      -2.914198    -0.048906    -0.993263      47.45
 H      -3.674363     0.375016    -1.648845      22.45
 C      -2.146479     1.171910    -0.651786      -4.99
 O      -2.771712     2.317624    -0.627298     161.84
 C      -4.228556     2.470694    -0.901191     105.83
 H      -4.851239     1.576097    -0.684407      22.97
 H      -4.613196     3.600532    -1.228439      21.26
 H      -4.482379     2.171082    -2.188077      22.20
 C      -0.744831     1.070398    -0.429553      19.61
 O      -0.358590     2.260259     0.316196     104.00
 C      -0.267733    -0.170028    -0.268640      39.96
 H       0.854733    -0.257974     0.059948      18.05
 C      -2.283305    -1.335002    -0.808793     -23.28
 C      -3.211480    -2.661952    -0.933482      94.35
 H      -4.061425    -2.202869    -1.295910      22.81
 O      -2.529917    -3.474451    -1.913433     255.65
 H      -2.790688    -4.450193    -1.954582      20.76
 C      -3.578973    -3.420094     0.268319      96.45
 H      -2.841275    -3.961752     0.743359      22.91
 O      -4.463279    -2.343060     1.122299     203.99
 H      -4.778020    -2.414128     2.187013      24.62
 C      -4.678267    -4.473449    -0.020246     100.80
 O      -4.162737    -5.662656    -0.741753     290.85
 H      -3.812920    -6.295726    -0.175087      32.20
 H      -5.578339    -4.005973    -0.582488      26.58
 H      -5.309420    -4.998049     0.800288      26.10
55
name = lig-etoh-frame_919
 C       2.584139     1.790211    -2.464773      52.05
 H       2.201144     2.177544    -3.396681      19.05
 C       3.482558     1.550073    -0.317299      69.13
 H       3.225498     1.686112     0.805234      15.44
 C       4.195639     0.302876    -0.763829       9.27
 O       4.748909    -0.707611     0.164508     257.57
 C       5.806250    -0.070164     1.083296     103.20
 H       5.128386     0.462756     1.839421      26.51
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 H       6.213470     0.712159     0.471602      28.58
 H       6.409332    -0.739256     1.617134      27.42
 C       4.110095    -0.165793    -2.066325       7.71
 O       5.035078    -1.243114    -2.584895     230.52
 H       5.171220    -1.852267    -1.918019      27.21
 C       3.263952     0.585272    -2.883501      45.27
 H       3.156643     0.496574    -3.876369      27.66
 C       2.467264     2.121983    -1.110964      72.62
 C       1.785050     3.328548    -0.649969      98.89
 H       1.779907     4.176652    -1.431970      21.62
 O       2.174340     3.669020     0.795076     338.59
 H       2.845560     4.213031     1.225859      34.37
 C       0.133299     3.445006    -0.640932      76.01
 H      -0.068482     3.185016    -1.653023      21.05
 C      -0.439124     4.724014     0.005666      99.48
 O      -0.017484     5.913577    -0.591988     303.25
 H      -0.130745     5.812810    -1.557625      32.07
 H      -0.008596     4.535029     1.011372      23.34
 H      -1.594528     4.520668    -0.050585      21.88
 C      -0.885512    -1.449227    -0.420306      27.89
 H      -0.615368    -2.506522     0.083439      19.89
 C      -2.884296    -0.065925    -1.002039      63.21
 H      -3.816591     0.140222    -1.624732      23.50
 C      -2.163217     1.108959    -0.691240      -3.92
 O      -2.867670     2.376882    -0.593748     180.80
 C      -4.197750     2.500240    -0.967994     129.14
 H      -5.126690     1.868854    -0.463084      24.65
 H      -4.625975     3.413040    -0.696796      26.28
 H      -4.284931     2.137895    -1.928695      27.42
 C      -0.773258     1.113306    -0.411291       9.20
 O      -0.308694     2.279649     0.281462     135.44
 C      -0.228996    -0.177618    -0.256771      30.47
 H       0.678017    -0.272964     0.219904      20.58
 C      -2.315771    -1.316243    -0.788724     -22.60
 C      -3.175073    -2.668950    -0.956728      72.22
 H      -4.223255    -2.356398    -1.590408      19.06
 O      -2.521696    -3.512786    -1.880564     254.17
 H      -2.932478    -4.367282    -1.816233      21.14
 C      -3.554756    -3.362215     0.319088      89.69
 H      -2.814342    -4.003527     0.962428      18.74
 O      -4.440344    -2.374970     1.110659     275.71
 H      -4.409844    -2.628555     2.060812      26.20
 C      -4.735051    -4.514002     0.014623      88.18
 O      -4.117430    -5.660343    -0.717011     275.19
 H      -3.640594    -6.386556    -0.127928      26.73
 H      -5.593156    -4.066263    -0.520153      27.80
 H      -5.080903    -4.963665     0.927095      27.91
55
name = lig-etoh-frame_920
 C       2.605155     1.778506    -2.483299      53.12
 H       2.170456     2.350848    -3.331242      16.75
 C       3.490289     1.505321    -0.324225      73.34
 H       3.609635     1.752622     0.688328      17.61
 C       4.176162     0.251961    -0.713446      24.37
 O       4.722559    -0.701878     0.153162     267.97
 C       5.808957    -0.088140     1.040155      90.06
 H       5.318282     0.397788     1.881162      26.91
 H       6.266695     0.850633     0.588313      27.64
 H       6.377966    -1.081094     1.425084      23.94
 C       4.115259    -0.176307    -1.991530       4.67
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 O       5.017826    -1.201575    -2.596734     160.43
 H       5.397740    -1.818354    -1.715588      21.30
 C       3.253826     0.631107    -2.884011      47.22
 H       3.209887     0.391471    -4.061245      25.51
 C       2.526190     2.127921    -1.106726      54.82
 C       1.805988     3.376449    -0.691347      92.62
 H       1.963068     4.317237    -1.256999      22.85
 O       2.158126     3.654381     0.787212     281.30
 H       3.160503     3.915293     0.999569      28.98
 C       0.109288     3.338074    -0.623861      78.13
 H      -0.308987     3.023380    -1.653521      20.54
 C      -0.444196     4.669283     0.061391      99.90
 O      -0.053785     5.883762    -0.588100     308.63
 H       0.005331     5.715083    -1.559777      31.15
 H      -0.098217     4.731873     1.107192      24.71
 H      -1.460782     4.394614     0.004204      24.50
 C      -0.973988    -1.447640    -0.378374      26.53
 H      -0.375249    -2.327946    -0.229504      19.35
 C      -2.864608    -0.073449    -1.038359      63.98
 H      -3.900044    -0.288928    -1.308846      23.14
 C      -2.211418     1.079090    -0.741749       2.73
 O      -2.924088     2.424655    -0.542293     143.70
 C      -4.245262     2.494269    -1.000581      97.90
 H      -4.852196     2.132245    -0.182735      24.01
 H      -4.414271     3.544311    -0.373913      21.04
 H      -4.257245     2.216101    -2.269972      20.95
 C      -0.852283     1.169601    -0.351757     -24.10
 O      -0.251077     2.290772     0.219258     187.26
 C      -0.163382    -0.230677    -0.222492     -34.72
 H       0.822512    -0.192540     0.413439      16.94
 C      -2.321763    -1.361127    -0.773277      15.76
 C      -3.155163    -2.609843    -1.021865      82.11
 H      -4.086151    -2.467404    -1.444255      24.32
 O      -2.486863    -3.563783    -1.858393     208.28
 H      -3.155045    -4.442157    -1.620055      14.45
 C      -3.645560    -3.342059     0.416654      79.21
 H      -2.750720    -3.634222     0.985594      22.43
 O      -4.381935    -2.420478     1.089653     338.15
 H      -4.079338    -2.708392     1.980983      24.32
 C      -4.725621    -4.570812     0.066384      76.30
 O      -4.090013    -5.655694    -0.715310     301.88
 H      -3.419747    -6.111921    -0.091817      25.93
 H      -5.541582    -4.172593    -0.573774      26.93
 H      -4.928561    -4.763435     1.185515      26.59
55
name = lig-etoh-frame_921
 C       2.599712     1.759669    -2.511547      27.55
 H       2.043371     2.564725    -2.998999      15.54
 C       3.503423     1.394998    -0.290122      73.19
 H       3.978500     1.880877     0.672860      19.67
 C       4.123376     0.221628    -0.630015      27.44
 O       4.731563    -0.666667     0.164354     270.35
 C       5.780144    -0.124600     1.009520     125.57
 H       5.436249     0.212816     2.041758      25.81
 H       6.494805     0.589510     0.585440      28.47
 H       6.375949    -0.946390     1.081418      27.69
 C       4.118807    -0.193959    -2.028606       8.44
 O       4.960619    -1.153001    -2.562681     231.83
 H       5.484466    -1.527697    -1.868907      25.71
 C       3.291670     0.631812    -2.923933      55.73
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 H       3.372899     0.271200    -3.889251      26.53
 C       2.623977     2.160442    -1.141629      58.72
 C       1.791168     3.456990    -0.659336     105.32
 H       2.365147     4.367334    -1.150606      20.57
 O       2.145402     3.640452     0.764901     326.72
 H       3.071367     3.650691     0.494440      28.07
 C       0.159151     3.257072    -0.634847      86.16
 H      -0.421069     3.219854    -1.535922      19.90
 C      -0.438202     4.579839     0.098441      82.47
 O      -0.092728     5.863513    -0.589241     256.34
 H       0.160031     5.587262    -1.619114      27.69
 H      -0.187384     4.876630     1.136583      22.91
 H      -1.611664     4.499697     0.121405      22.18
 C      -0.999148    -1.390274    -0.334431      42.65
 H      -0.313981    -2.294172    -0.461991      19.63
 C      -2.884878    -0.144880    -1.077348      34.87
 H      -4.014601    -0.311810    -0.942337      22.96
 C      -2.268676     1.160412    -0.761299      -8.78
 O      -2.913330     2.414073    -0.503091     164.51
 C      -4.305159     2.551805    -0.983195     116.52
 H      -4.845462     1.790480    -0.260205      23.34
 H      -4.301266     3.614609    -0.929372      25.05
 H      -4.606553     2.542124    -1.926007      27.58
 C      -0.901373     1.114950    -0.270853     -18.22
 O      -0.210853     2.251944     0.183598     198.50
 C      -0.157476    -0.226231    -0.161715       6.64
 H       0.813959    -0.203371     0.268935      19.63
 C      -2.307642    -1.413282    -0.783518      17.90
 C      -3.131058    -2.579435    -1.035871      57.49
 H      -4.271455    -2.241607    -1.440041      19.57
 O      -2.465950    -3.640759    -1.826919     232.90
 H      -2.934815    -4.392775    -1.677005      23.05
 C      -3.723027    -3.347912     0.402287      75.13
 H      -2.695247    -3.474325     0.920621      20.31
 O      -4.340842    -2.441965     1.112416     315.16
 H      -3.995191    -2.317478     2.195571      22.26
 C      -4.640434    -4.602301     0.144300      87.72
 O      -4.067222    -5.643605    -0.698888     349.88
 H      -3.251846    -5.894239    -0.236184      29.75
 H      -5.544350    -4.293774    -0.498119      24.89
 H      -5.054138    -4.792734     1.141454      26.12
55
name = lig-etoh-frame_922
 C       2.573505     1.772111    -2.495015      41.50
 H       1.904299     2.502300    -3.043052      20.39
 C       3.509191     1.349243    -0.209801      76.26
 H       3.956673     1.827167     0.585499      25.47
 C       4.050219     0.169210    -0.644338      17.25
 O       4.767378    -0.635206     0.201994     269.49
 C       5.770489    -0.170710     1.003773     114.78
 H       5.534781    -0.000750     2.070173      25.66
 H       6.469019     0.497774     0.451274      26.08
 H       6.580349    -1.084442     0.991553      24.04
 C       4.081220    -0.154298    -2.066093      21.48
 O       4.886223    -1.106738    -2.535493     192.38
 H       5.555725    -1.403405    -1.856924      22.86
 C       3.370259     0.588717    -2.958491      55.17
 H       3.456713     0.223603    -4.059437      21.33
 C       2.733912     2.183160    -1.175520      79.18
 C       1.796860     3.495481    -0.614516     123.92
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 H       2.229681     4.289493    -1.189515      21.04
 O       2.136561     3.625121     0.720637     360.49
 H       3.105593     3.583867     0.565128      29.33
 C       0.231243     3.298076    -0.651638      73.30
 H      -0.308107     3.405018    -1.640039      16.81
 C      -0.456183     4.530699     0.115475      92.24
 O      -0.122672     5.823383    -0.611395     299.50
 H       0.113917     5.605743    -1.460474      36.11
 H      -0.099402     4.681238     1.152856      24.15
 H      -1.509678     4.542943     0.144303      24.59
 C      -0.921087    -1.346517    -0.305214      51.23
 H      -0.481351    -2.367740    -0.497197      19.55
 C      -2.944867    -0.179209    -1.063817      19.89
 H      -3.983139    -0.019496    -0.918835      22.28
 C      -2.303258     1.208880    -0.739587     -18.56
 O      -2.886714     2.369467    -0.507212     138.88
 C      -4.347413     2.625251    -0.889896     102.07
 H      -5.018796     1.802572    -0.627917      22.28
 H      -4.553953     3.760664    -1.130274      21.28
 H      -4.871140     2.446541    -2.125754      21.10
 C      -0.918763     1.001159    -0.206275      10.63
 O      -0.183607     2.148429     0.192312     146.19
 C      -0.256074    -0.161606    -0.102745      64.26
 H       0.869721    -0.257094     0.069351      20.25
 C      -2.281635    -1.406883    -0.816977      -0.55
 C      -3.188119    -2.630189    -1.025465      75.37
 H      -3.950687    -2.154931    -1.529518      20.40
 O      -2.435994    -3.676655    -1.798212     186.13
 H      -2.928504    -4.625719    -1.709013      16.77
 C      -3.689940    -3.375961     0.322111      84.98
 H      -2.720267    -3.740358     0.745626      21.69
 O      -4.351610    -2.387773     1.207864     415.11
 H      -4.152408    -2.135336     2.018111      34.87
 C      -4.567485    -4.600876     0.197537     106.84
 O      -4.043506    -5.627885    -0.666152     308.07
 H      -3.039538    -5.943520    -0.411810      24.46
 H      -5.477183    -4.297367    -0.300771      24.79
 H      -5.104962    -5.091972     1.095032      24.90
55
name = lig-etoh-frame_923
 C       2.571979     1.761649    -2.482989      93.92
 H       1.941142     2.157234    -3.248071      25.74
 C       3.483699     1.366821    -0.181029      84.50
 H       3.803949     1.745800     0.885258      20.04
 C       3.988778     0.128099    -0.682018       2.09
 O       4.775535    -0.645640     0.217726     271.91
 C       5.866051    -0.249874     1.006310     103.67
 H       5.561453    -0.004278     2.047961      26.40
 H       6.205745     0.716781     0.511076      26.21
 H       6.473950    -1.053747     1.133057      26.64
 C       4.033673    -0.101534    -2.050181      23.55
 O       4.829680    -1.101016    -2.526442     147.67
 H       5.596997    -1.360468    -1.753056      20.79
 C       3.390266     0.601370    -3.023363      53.27
 H       3.445168     0.386579    -4.096323      25.41
 C       2.807443     2.198503    -1.171985      55.67
 C       1.824259     3.453019    -0.609257     124.05
 H       1.839356     4.397483    -1.388946      17.78
 O       2.152815     3.621132     0.699801     353.39
 H       3.085909     3.724580     1.101893      28.02
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 C       0.265939     3.383658    -0.649025      57.40
 H       0.017024     3.249738    -1.709182      17.35
 C      -0.439852     4.524130     0.110874      90.11
 O      -0.153538     5.778570    -0.602832     248.98
 H       0.058813     5.552468    -1.644634      26.30
 H       0.047781     4.410028     1.099703      21.98
 H      -1.580730     4.339607     0.107291      21.51
 C      -0.895277    -1.381394    -0.332529      54.38
 H      -0.422610    -2.343704    -0.273285      21.61
 C      -2.982896    -0.107830    -0.999106      22.85
 H      -4.120501     0.063190    -1.189143      21.91
 C      -2.288762     1.098118    -0.689250       3.28
 O      -2.909824     2.363668    -0.538754     145.71
 C      -4.394842     2.681833    -0.898530     106.86
 H      -5.227856     2.067705    -0.453432      25.00
 H      -4.749460     3.692127    -0.660703      24.74
 H      -4.397224     2.249850    -1.953549      22.20
 C      -0.975628     1.008643    -0.186574       1.29
 O      -0.150000     2.043201     0.210638      61.14
 C      -0.314557    -0.158262    -0.040139      74.55
 H       0.789399    -0.125106    -0.107226      22.21
 C      -2.252744    -1.364808    -0.831809     -38.83
 C      -3.221991    -2.728684    -0.994776      70.41
 H      -3.957224    -2.241989    -1.871613      16.48
 O      -2.409905    -3.699373    -1.770786     188.25
 H      -3.003710    -4.567773    -1.750808      17.83
 C      -3.616053    -3.368463     0.298251      84.00
 H      -2.708686    -3.903119     0.672318      20.90
 O      -4.392094    -2.332780     1.233586     255.67
 H      -3.998698    -2.237909     2.348321      21.75
 C      -4.547110    -4.603547     0.231184      98.50
 O      -3.997964    -5.619241    -0.656919     346.73
 H      -3.243266    -6.076150    -0.310241      29.63
 H      -5.533621    -4.207848    -0.266056      24.37
 H      -4.755024    -5.186783     1.133450      26.56
55
name = lig-etoh-frame_924
 C       2.629090     1.695809    -2.503018      53.03
 H       1.904416     2.087412    -3.282144      24.03
 C       3.462137     1.401961    -0.187715      94.80
 H       3.389039     1.489372     0.877813      20.01
 C       3.961438     0.155823    -0.635577      20.26
 O       4.743350    -0.706425     0.195644     265.80
 C       5.947862    -0.258006     1.020592      80.53
 H       5.500404     0.067485     2.014638      26.65
 H       6.219331     0.757141     0.744451      27.24
 H       6.666134    -1.191803     1.186679      24.27
 C       4.017946    -0.098607    -2.050493      12.73
 O       4.808325    -1.128324    -2.511959     195.80
 H       5.319939    -1.394362    -1.837435      24.98
 C       3.336291     0.698512    -3.052771      39.18
 H       3.421660     0.494756    -4.116258      25.12
 C       2.797544     2.232232    -1.141801      57.06
 C       1.878368     3.394665    -0.654342     120.48
 H       1.863755     4.272116    -1.245712      20.13
 O       2.174309     3.638095     0.740083     347.30
 H       2.913391     4.019481     1.244874      31.98
 C       0.296155     3.390629    -0.639842      43.84
 H       0.133977     3.019476    -1.665742      20.14
 C      -0.420327     4.507185     0.070978     104.64
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 O      -0.175847     5.737407    -0.594475     304.35
 H      -0.151680     5.520896    -1.579564      28.95
 H       0.060099     4.459991     1.063975      22.22
 H      -1.432390     4.126363     0.135944      23.18
 C      -0.942495    -1.447437    -0.388769      37.61
 H      -0.259766    -2.321200     0.018726      22.95
 C      -3.009073    -0.047986    -0.927283      72.61
 H      -3.912602    -0.124307    -1.432931      22.53
 C      -2.314719     0.997773    -0.616067      29.12
 O      -2.954845     2.383409    -0.559419     152.76
 C      -4.439144     2.673091    -0.910512     102.10
 H      -5.120466     2.254185    -0.114664      24.23
 H      -4.553475     3.698558    -0.434688      23.89
 H      -3.989208     2.337766    -1.976322      17.73
 C      -1.015864     1.084360    -0.181346      -3.63
 O      -0.110896     1.991178     0.225162      35.92
 C      -0.322978    -0.218878    -0.011770      -0.19
 H       0.744876     0.018368     0.023262      20.05
 C      -2.279027    -1.344232    -0.830059     -13.34
 C      -3.199346    -2.758855    -1.037743      91.50
 H      -4.037289    -2.647118    -1.636609      25.21
 O      -2.391038    -3.720028    -1.741773     252.02
 H      -2.957426    -4.466283    -1.750551      22.74
 C      -3.584341    -3.346269     0.350355      75.54
 H      -2.568995    -3.705788     0.797938      21.18
 O      -4.394103    -2.294533     1.255467     292.73
 H      -4.100690    -2.675381     2.053044      26.86
 C      -4.549088    -4.592593     0.226017     103.00
 O      -3.967187    -5.611854    -0.679662     314.86
 H      -3.374277    -6.247849    -0.024789      24.60
 H      -5.480529    -4.319780    -0.139676      28.79
 H      -4.525365    -4.885216     1.263921      29.00
55
name = lig-etoh-frame_925
 C       2.641053     1.724383    -2.502370      43.19
 H       1.934555     2.332011    -3.003365      23.82
 C       3.416306     1.419618    -0.207965      72.62
 H       3.057620     1.476605     0.855816      19.40
 C       3.984719     0.206756    -0.594910      22.40
 O       4.714070    -0.780511     0.165947     217.48
 C       5.964339    -0.244656     1.058569      90.98
 H       5.514477    -0.092356     2.011215      27.65
 H       6.551384     0.667512     0.708342      27.21
 H       6.718477    -0.994286     1.072225      27.46
 C       4.020638    -0.112274    -2.068478       6.47
 O       4.777958    -1.159693    -2.517522     139.67
 H       5.227166    -1.649816    -1.630955      19.51
 C       3.329385     0.723942    -3.031674      48.47
 H       3.345333     0.500401    -4.172581      21.85
 C       2.730544     2.233578    -1.135719      63.92
 C       1.938204     3.353936    -0.646662     117.33
 H       2.313835     4.357249    -1.244278      19.13
 O       2.178219     3.658670     0.809797     286.03
 H       2.902225     4.361785     0.917177      29.75
 C       0.355670     3.274767    -0.640297      57.30
 H      -0.107273     2.999795    -1.632953      21.31
 C      -0.385478     4.456100     0.034506      94.76
 O      -0.202798     5.713794    -0.589974     297.04
 H      -0.299069     5.560246    -1.532163      31.30
 H      -0.015441     4.712469     1.049241      22.92
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 H      -1.462810     4.117461     0.148597      23.06
 C      -0.974938    -1.487049    -0.401757      60.43
 H      -0.494213    -2.325532    -0.070612      27.82
 C      -3.021010    -0.151847    -0.887639      64.71
 H      -3.915974    -0.192351    -1.615899      21.09
 C      -2.381255     1.098233    -0.515182       5.38
 O      -2.975525     2.388424    -0.551903     150.82
 C      -4.414115     2.654807    -0.886416     108.97
 H      -5.008475     2.022779    -0.216130      24.95
 H      -4.174041     3.776443    -0.791335      23.30
 H      -4.568775     2.639428    -2.008545      24.90
 C      -0.969031     1.052760    -0.160211       0.07
 O      -0.067542     2.017949     0.239541     102.63
 C      -0.357683    -0.246815    -0.040351       5.10
 H       0.722811    -0.106229     0.404143      19.46
 C      -2.369804    -1.380391    -0.835312      -4.92
 C      -3.132434    -2.732436    -1.064192      82.54
 H      -4.335570    -2.784110    -1.410332      22.34
 O      -2.354035    -3.727117    -1.717879     192.84
 H      -2.935980    -4.686194    -1.722745      15.11
 C      -3.582855    -3.291661     0.407413      78.94
 H      -2.657049    -3.396580     0.988072      22.85
 O      -4.361559    -2.302169     1.223987     270.04
 H      -4.308901    -2.806703     2.130888      25.48
 C      -4.501755    -4.563419     0.218508      86.41
 O      -3.943644    -5.613385    -0.682383     284.86
 H      -3.536642    -6.296829    -0.039545      26.31
 H      -5.651193    -4.390847    -0.061449      26.65
 H      -4.658752    -4.765114     1.357353      27.43
55
name = lig-etoh-frame_926
 C       2.596258     1.874093    -2.449978      92.86
 H       1.973554     2.635908    -3.037061      21.78
 C       3.344346     1.405921    -0.193346      56.65
 H       3.013968     1.676967     0.839202      17.88
 C       4.047361     0.229508    -0.629991      19.12
 O       4.709893    -0.822280     0.148701     202.44
 C       5.943265    -0.223430     1.065598      86.82
 H       5.549914    -0.212496     2.158795      24.55
 H       6.512687     0.536030     0.579081      26.65
 H       6.708763    -1.079394     1.000013      25.30
 C       4.034442    -0.111909    -2.058257      21.83
 O       4.757939    -1.206000    -2.509736     188.11
 H       4.935327    -1.809370    -1.680558      22.82
 C       3.369515     0.663675    -3.009013      58.60
 H       3.278848     0.463064    -4.011898      24.99
 C       2.675348     2.158481    -1.150724      36.96
 C       1.979203     3.393964    -0.598056     114.42
 H       2.432237     4.139374    -1.137154      23.57
 O       2.201851     3.688774     0.868592     296.87
 H       2.740944     4.454985     0.538745      27.99
 C       0.392714     3.123742    -0.645917      79.20
 H      -0.196254     3.112149    -1.559795      20.69
 C      -0.356427     4.395607     0.029853      85.01
 O      -0.228052     5.706122    -0.601237     242.76
 H      -0.403727     5.665915    -1.681624      27.23
 H      -0.062667     4.701120     1.043682      23.57
 H      -1.451720     4.226664     0.061060      23.05
 C      -1.037948    -1.466992    -0.392937      54.21
 H      -0.693640    -2.613078    -0.275760      22.62
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 C      -3.043306    -0.238673    -0.887250      28.72
 H      -3.920323    -0.076990    -1.452445      25.67
 C      -2.428720     1.209484    -0.423512     -10.80
 O      -2.980082     2.372139    -0.547928     151.27
 C      -4.328114     2.662430    -0.898563     119.25
 H      -5.042137     1.939468    -0.389334      23.23
 H      -4.321028     3.746406    -0.898493      24.83
 H      -5.267553     2.693073    -1.739901      21.37
 C      -0.928716     0.979651    -0.144768     -20.16
 O      -0.018920     2.085349     0.258507     130.68
 C      -0.386288    -0.276834    -0.069764      73.54
 H       0.453552    -0.433890     0.535439      22.84
 C      -2.429698    -1.470089    -0.840522      24.89
 C      -3.135596    -2.711658    -1.037029     102.34
 H      -4.046189    -2.512648    -1.438297      26.65
 O      -2.316524    -3.742395    -1.707250     243.94
 H      -2.713807    -4.555334    -1.542098      22.03
 C      -3.586979    -3.216797     0.442776      84.86
 H      -2.679412    -3.379924     1.170002      22.27
 O      -4.320579    -2.337120     1.171560     286.03
 H      -4.643866    -2.460343     2.186745      26.05
 C      -4.468187    -4.525989     0.246933     107.72
 O      -3.944887    -5.610663    -0.661444     320.70
 H      -3.464214    -6.276473    -0.202628      30.64
 H      -5.411571    -4.303413    -0.114950      29.24
 H      -4.740691    -5.016877     1.178198      28.66
55
name = lig-etoh-frame_927
 C       2.580455     1.979717    -2.485278     114.54
 H       2.180865     2.636007    -3.203397      24.30
 C       3.294859     1.324283    -0.160068      35.76
 H       3.286491     1.747653     0.848759      19.33
 C       4.108355     0.237143    -0.670518      21.11
 O       4.726918    -0.809103     0.148597     226.86
 C       5.895034    -0.276123     1.051641      94.65
 H       5.648103    -0.077069     2.051005      26.85
 H       6.176388     0.697550     0.516261      24.92
 H       6.510594    -1.199689     0.995273      24.42
 C       4.060362    -0.111558    -2.033773      19.79
 O       4.728249    -1.264822    -2.497853     208.11
 H       4.807471    -1.833178    -1.794987      28.10
 C       3.352524     0.681186    -2.936337      59.22
 H       3.271374     0.308610    -4.073401      22.34
 C       2.625429     2.100152    -1.100402      18.56
 C       1.956472     3.381125    -0.520938      94.45
 H       2.311145     4.303257    -1.263761      21.50
 O       2.240908     3.725537     0.875043     297.16
 H       2.720141     4.593346     0.844276      27.75
 C       0.392241     3.072276    -0.631801      82.62
 H      -0.008584     3.020398    -1.702450      19.80
 C      -0.345057     4.363367     0.021171      84.20
 O      -0.245299     5.710231    -0.640239     299.49
 H      -0.342766     5.619962    -1.561366      31.28
 H       0.000886     4.414270     1.072780      23.06
 H      -1.418917     4.138089    -0.018807      22.58
 C      -1.145685    -1.493681    -0.391653      78.50
 H      -0.702493    -2.421791    -0.439267      24.20
 C      -3.061339    -0.193273    -0.879088      15.15
 H      -4.128357    -0.015377    -1.239400      25.31
 C      -2.385404     1.126168    -0.371217     -17.27
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 O      -2.980431     2.384226    -0.572242     174.24
 C      -4.341570     2.679150    -0.914981     126.17
 H      -4.924556     2.192182    -0.100301      26.51
 H      -4.647015     3.748586    -0.533382      24.71
 H      -4.934968     2.363741    -1.774858      26.55
 C      -0.950057     0.994326    -0.135020     -28.58
 O       0.013994     2.110369     0.285435     136.66
 C      -0.411753    -0.352695    -0.082077      38.56
 H       0.521104    -0.645553     0.567918      21.36
 C      -2.409078    -1.502201    -0.828993      34.91
 C      -3.155872    -2.736592    -0.971022      79.89
 H      -4.014718    -2.281560    -1.808719      20.97
 O      -2.276940    -3.720697    -1.694131     165.36
 H      -2.702823    -4.659319    -1.311845      13.51
 C      -3.557289    -3.225195     0.495955      96.44
 H      -2.639954    -3.561523     0.981204      24.57
 O      -4.338573    -2.305797     1.116875     344.00
 H      -4.524359    -2.342004     1.994415      31.25
 C      -4.419912    -4.519514     0.285017      88.76
 O      -3.962737    -5.588796    -0.649259     264.46
 H      -3.146714    -6.238517    -0.205214      22.63
 H      -5.309256    -4.039599    -0.372263      24.20
 H      -4.714459    -5.240703     1.132368      25.48
55
name = lig-etoh-frame_928
 C       2.644319     1.950982    -2.538851      33.73
 H       2.277072     2.643248    -3.326419      19.34
 C       3.287992     1.202117    -0.140684      42.33
 H       3.670136     1.626315     0.861455      20.73
 C       4.146689     0.222745    -0.656764      26.60
 O       4.745343    -0.757149     0.159839     266.55
 C       5.812049    -0.338641     0.985715     114.87
 H       5.539915     0.078515     2.069368      24.79
 H       6.044070     0.644458     0.606027      26.28
 H       6.527077    -1.148118     1.009845      25.72
 C       4.084910    -0.120770    -2.021723       6.85
 O       4.684522    -1.304396    -2.504430     162.27
 H       4.829087    -1.999215    -1.619728      20.47
 C       3.280610     0.764518    -2.889884      46.00
 H       3.329884     0.343467    -3.813468      25.44
 C       2.573924     2.114117    -1.022159      41.98
 C       1.913952     3.369483    -0.476206     107.32
 H       1.918199     4.166578    -1.102243      23.78
 O       2.286008     3.763422     0.861507     349.89
 H       2.737865     4.526612     1.271723      29.46
 C       0.384158     3.150182    -0.629057      73.76
 H       0.316124     2.755380    -1.651123      19.26
 C      -0.357949     4.345575    -0.018406      88.87
 O      -0.246498     5.704339    -0.649152     287.17
 H      -0.210471     5.445605    -1.670187      25.98
 H       0.062743     4.260189     0.998599      21.56
 H      -1.427625     3.961949    -0.011841      20.06
 C      -1.181797    -1.525653    -0.386784      61.05
 H      -0.482719    -2.453603    -0.420515      22.40
 C      -3.061457    -0.092725    -0.846607      59.84
 H      -4.144292    -0.082512    -0.915784      25.38
 C      -2.343336     0.968333    -0.390531     -10.47
 O      -2.949143     2.407185    -0.604231     126.94
 C      -4.423905     2.678609    -0.851308     104.04
 H      -4.849879     2.293020     0.125672      24.84
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 H      -4.596432     3.667971    -0.564396      25.39
 H      -4.201144     2.080535    -1.956428      18.91
 C      -0.956158     1.017207    -0.104968     -33.46
 O       0.002525     2.054119     0.315979     102.04
 C      -0.424768    -0.403772    -0.055780      18.65
 H       0.577408    -0.479606     0.224825      24.65
 C      -2.454245    -1.416184    -0.819627      10.08
 C      -3.194550    -2.760222    -0.964813      96.94
 H      -3.899486    -2.624963    -1.645152      25.09
 O      -2.261643    -3.700561    -1.654192     201.59
 H      -2.635835    -4.594122    -1.336137      17.46
 C      -3.523934    -3.314638     0.510293      78.92
 H      -2.432664    -3.594898     0.856471      22.45
 O      -4.378936    -2.226487     1.046152     291.63
 H      -4.221428    -2.409688     2.163241      23.05
 C      -4.413102    -4.541407     0.289643     109.61
 O      -3.938080    -5.577316    -0.642274     374.39
 H      -3.211533    -5.928230    -0.226221      33.45
 H      -5.139578    -4.064383    -0.255941      28.02
 H      -4.772923    -4.949119     1.202310      28.75
55
name = lig-etoh-frame_929
 C       2.711974     1.902276    -2.490085      35.08
 H       2.250772     2.594813    -3.185433      20.63
 C       3.306164     1.149774    -0.134770      44.95
 H       3.635330     1.390061     0.829219      22.47
 C       4.156152     0.167679    -0.650312      29.96
 O       4.741893    -0.721801     0.162714     296.19
 C       5.730057    -0.344126     0.962168     126.73
 H       5.340202    -0.151473     1.915019      27.83
 H       6.341942     0.564064     0.573609      26.02
 H       6.690525    -0.999488     1.086386      25.15
 C       4.078229    -0.118620    -2.013160      12.21
 O       4.627673    -1.341523    -2.499948     220.21
 H       4.923274    -1.797654    -1.709487      24.62
 C       3.264563     0.780273    -2.847378      52.95
 H       3.314459     0.468453    -3.988027      24.39
 C       2.574062     2.136698    -0.979497      42.55
 C       1.871381     3.368715    -0.417958      95.85
 H       1.846959     4.313747    -1.240799      19.10
 O       2.310783     3.765410     0.865165     313.84
 H       2.908264     4.491665     1.244798      26.85
 C       0.388013     3.222328    -0.608261      53.26
 H       0.385171     2.654587    -1.568938      17.26
 C      -0.409873     4.328474    -0.071501     100.79
 O      -0.244360     5.665570    -0.658210     289.20
 H       0.043134     5.431169    -1.654040      25.26
 H       0.038883     4.450020     0.935061      21.76
 H      -1.420727     4.013671     0.024823      22.15
 C      -1.116008    -1.548218    -0.374145      -1.91
 H      -0.579679    -2.512268    -0.353052      22.36
 C      -3.080057    -0.080178    -0.801158      90.24
 H      -4.152929    -0.029279    -0.705344      23.49
 C      -2.314368     0.970777    -0.443685      -5.01
 O      -2.873257     2.415033    -0.603173      99.92
 C      -4.433166     2.604530    -0.776420     108.66
 H      -5.062386     2.021489    -0.071001      25.11
 H      -4.421076     3.812413    -1.062338      23.04
 H      -4.337922     2.262813    -1.678064      25.89
 C      -0.915394     0.960055    -0.056123      -8.06
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 O      -0.052618     1.958681     0.330348      73.27
 C      -0.434356    -0.361428    -0.024903      28.78
 H       0.744978    -0.317101    -0.115217      22.21
 C      -2.559880    -1.330746    -0.812744     -22.68
 C      -3.181804    -2.778373    -0.957988      58.27
 H      -4.350277    -2.964562    -1.555223      21.22
 O      -2.246309    -3.673374    -1.607597     209.64
 H      -2.603434    -4.546420    -1.509837      19.50
 C      -3.484301    -3.382370     0.446522      91.88
 H      -2.550969    -3.410679     0.988691      23.28
 O      -4.391363    -2.180468     1.031359     326.58
 H      -4.017883    -2.212841     1.924988      27.48
 C      -4.422219    -4.562361     0.288949      85.90
 O      -3.915985    -5.552383    -0.632426     323.34
 H      -3.066653    -6.039662    -0.093502      24.20
 H      -5.428280    -4.131973    -0.193091      25.27
 H      -4.900575    -4.715161     1.355068      26.18
55
name = lig-etoh-frame_930
 C       2.717439     1.926131    -2.315371      71.31
 H       2.184783     2.564162    -3.017413      18.41
 C       3.320072     1.188340    -0.151798      47.67
 H       3.266829     1.261120     1.037554      18.71
 C       4.109624     0.129612    -0.683544      25.58
 O       4.718171    -0.755452     0.133671     287.35
 C       5.762499    -0.290121     0.999536     113.45
 H       5.217967    -0.261188     2.032327      25.14
 H       6.379246     0.493136     0.622342      28.17
 H       6.479950    -1.075922     1.112701      26.59
 C       4.047206    -0.133782    -2.031606      28.59
 O       4.562306    -1.347320    -2.504470     201.63
 H       5.084290    -1.709116    -1.708295      22.92
 C       3.340694     0.668243    -2.880981      68.76
 H       3.254412     0.710395    -3.928097      31.11
 C       2.643637     2.121691    -0.965288      56.23
 C       1.865985     3.418560    -0.400994     124.89
 H       2.150158     4.124058    -1.095508      28.69
 O       2.317277     3.751495     0.899212     295.38
 H       3.088808     4.367017     0.720289      29.80
 C       0.392638     3.200670    -0.571302      47.64
 H       0.114083     2.911255    -1.594244      20.51
 C      -0.473604     4.350261    -0.086428      98.56
 O      -0.230144     5.613772    -0.690069     306.83
 H       0.096467     5.584199    -1.585740      31.01
 H      -0.126275     4.638628     0.928781      23.41
 H      -1.606869     4.137473    -0.004337      21.99
 C      -1.102260    -1.510665    -0.378984      10.20
 H      -0.740748    -2.549709    -0.353008      23.24
 C      -3.147372    -0.099320    -0.750596      27.55
 H      -4.255884     0.126062    -0.703401      22.43
 C      -2.266293     1.135124    -0.489434      -3.08
 O      -2.795295     2.391066    -0.567239      98.80
 C      -4.364985     2.560733    -0.722122      97.83
 H      -5.209822     1.997209    -0.270094      22.26
 H      -4.442267     3.467706    -1.135667      25.11
 H      -4.935023     2.106354    -1.959134      20.19
 C      -0.924629     0.884997    -0.026737      24.27
 O      -0.112329     1.884579     0.341185      69.61
 C      -0.372455    -0.334042    -0.023312      69.77
 H       0.659199    -0.337014    -0.180648      23.31
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 C      -2.568751    -1.376530    -0.783211     -14.37
 C      -3.221322    -2.802423    -0.969695     107.11
 H      -4.140232    -2.900169    -1.246523      27.17
 O      -2.212315    -3.627943    -1.575675     194.79
 H      -2.733890    -4.597674    -1.750425      16.71
 C      -3.493202    -3.360877     0.360982      95.14
 H      -2.742470    -3.358758     1.251160      21.52
 O      -4.372478    -2.174547     1.011392     310.27
 H      -4.047642    -1.978762     1.960674      27.96
 C      -4.486819    -4.543255     0.307725     102.12
 O      -3.874627    -5.545707    -0.592083     329.39
 H      -3.304809    -6.245312    -0.181867      27.76
 H      -5.419489    -4.315224    -0.138820      28.29
 H      -4.760565    -4.897713     1.270946      28.66
55
name = lig-etoh-frame_931
 C       2.728705     1.891726    -2.203736      89.95
 H       2.148386     2.564033    -2.873122      20.43
 C       3.346284     1.230237    -0.112479      71.23
 H       2.929870     1.188656     0.831205      21.93
 C       4.014346     0.148473    -0.682641      23.41
 O       4.706638    -0.825675     0.094646     219.70
 C       5.799764    -0.265284     1.084970      78.28
 H       5.377326    -0.034270     2.058143      27.57
 H       6.243025     0.714551     0.703797      25.93
 H       6.257854    -1.339034     1.118881      23.06
 C       4.021644    -0.202462    -2.087055      25.17
 O       4.504704    -1.355127    -2.503356     108.74
 H       5.343322    -1.664593    -1.828241      22.04
 C       3.374711     0.665517    -2.912737      71.81
 H       3.302874     0.655146    -4.025869      28.47
 C       2.713655     2.127390    -0.911231      59.29
 C       1.896554     3.398661    -0.405234     111.63
 H       2.440625     4.212820    -1.134519      24.32
 O       2.329596     3.757093     0.934051     297.10
 H       3.144479     4.063640     0.506889      29.40
 C       0.337094     3.140241    -0.529776      51.02
 H      -0.070746     3.171360    -1.573413      19.07
 C      -0.548224     4.393818    -0.046650      98.17
 O      -0.211403     5.592421    -0.723520     291.99
 H       0.051122     5.553015    -1.809895      25.38
 H      -0.377253     4.575005     1.029955      24.89
 H      -1.572146     4.199736    -0.178499      24.30
 C      -1.156011    -1.443790    -0.400689      54.87
 H      -0.749559    -2.537937    -0.387832      23.16
 C      -3.177946    -0.062576    -0.688546     -11.61
 H      -4.207631     0.103897    -0.864603      18.62
 C      -2.262695     1.190644    -0.530069       7.35
 O      -2.781771     2.381614    -0.527882     160.62
 C      -4.286198     2.462754    -0.789267     104.58
 H      -5.060140     2.147288     0.027883      23.74
 H      -4.528106     3.652672    -0.925819      23.29
 H      -4.865874     2.015677    -1.588639      22.94
 C      -0.997825     0.883482    -0.043076      15.82
 O      -0.129159     1.881839     0.359896      91.64
 C      -0.308430    -0.409084    -0.062474      49.98
 H       0.839722    -0.450044     0.025507      21.50
 C      -2.509361    -1.448299    -0.730862      16.10
 C      -3.193983    -2.786986    -0.951699      78.21
 H      -4.366028    -2.619568    -1.599142      21.17
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 O      -2.188542    -3.608597    -1.585898     234.75
 H      -2.668705    -4.360353    -1.795060      24.72
 C      -3.573083    -3.286577     0.407993     106.17
 H      -2.810622    -3.565432     1.075657      25.52
 O      -4.352253    -2.187889     0.975684     307.30
 H      -4.154385    -1.949369     2.022749      26.59
 C      -4.515879    -4.540487     0.328843      87.43
 O      -3.857032    -5.550657    -0.566495     306.45
 H      -3.397846    -6.289094    -0.096329      27.76
 H      -5.510406    -4.303588    -0.226435      25.38
 H      -4.584265    -5.163215     1.274304      26.26
55
name = lig-etoh-frame_932
 C       2.751669     1.807396    -2.255198      45.16
 H       2.196888     2.542146    -2.806876      24.31
 C       3.378464     1.228714    -0.032560      60.99
 H       2.881519     1.128519     1.010330      20.79
 C       3.943462     0.132119    -0.660312      12.68
 O       4.702938    -0.870643     0.069853     158.37
 C       5.796335    -0.281637     1.145808      88.07
 H       5.408224     0.158168     2.131827      25.90
 H       6.194152     0.639837     0.726428      26.47
 H       6.368392    -1.153219     1.208644      26.22
 C       3.977840    -0.230559    -2.097814      12.85
 O       4.498738    -1.409686    -2.511478     197.99
 H       5.222075    -1.613564    -2.066682      30.29
 C       3.350455     0.770901    -2.930100      51.22
 H       3.380271     0.472512    -4.012181      21.74
 C       2.745287     2.179878    -0.834023      39.37
 C       1.939795     3.340037    -0.432749     104.81
 H       2.114622     4.149258    -1.052602      23.58
 O       2.336918     3.765888     0.942699     278.32
 H       3.386242     3.921018     0.987231      28.12
 C       0.242707     3.118743    -0.474006      53.93
 H      -0.007950     3.007516    -1.542404      21.38
 C      -0.596769     4.420776     0.009636      93.34
 O      -0.177004     5.604173    -0.774939     304.25
 H      -0.159300     5.255279    -1.647721      29.91
 H      -0.599235     4.524314     1.114660      24.86
 H      -1.649871     4.133209    -0.379812      21.53
 C      -1.171979    -1.456305    -0.421179      52.96
 H      -0.677562    -2.358549    -0.433723      23.17
 C      -3.115119    -0.048187    -0.644044      44.25
 H      -4.181627    -0.028172    -1.041896      19.65
 C      -2.323828     1.062410    -0.555566      18.08
 O      -2.835321     2.420385    -0.504591     174.21
 C      -4.218540     2.456647    -0.804300     108.66
 H      -4.508254     2.247382     0.345036      23.02
 H      -4.422850     3.444600    -0.663887      25.54
 H      -4.553325     1.580069    -1.735956      19.78
 C      -0.989760     0.888827    -0.083865     -15.67
 O      -0.115401     1.940299     0.368388     113.33
 C      -0.288433    -0.442416    -0.122707      19.62
 H       0.700717    -0.577565     0.349412      22.18
 C      -2.494817    -1.397592    -0.678189      31.54
 C      -3.187417    -2.726422    -0.964856      96.08
 H      -3.801663    -2.477437    -1.691222      28.30
 O      -2.174969    -3.582299    -1.615661     209.41
 H      -2.654990    -4.475568    -1.791977      21.10
 C      -3.708144    -3.241855     0.502813      84.96
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 H      -2.628407    -3.697654     0.841437      22.27
 O      -4.348078    -2.188517     0.963934     350.09
 H      -4.191130    -2.232229     1.849525      31.39
 C      -4.521751    -4.572187     0.324070      96.34
 O      -3.859908    -5.547816    -0.566406     307.09
 H      -3.305444    -6.202265     0.123913      24.42
 H      -5.501205    -4.282754    -0.084636      27.03
 H      -4.691815    -5.046548     1.295935      27.90
55
name = lig-etoh-frame_933
 C       2.743454     1.809639    -2.305493      67.18
 H       2.240629     2.563299    -2.961297      26.22
 C       3.364543     1.217677     0.074716      48.57
 H       3.326898     1.158734     1.160636      21.70
 C       3.936561     0.041163    -0.646837      11.11
 O       4.711816    -0.885031     0.081704     180.24
 C       5.739730    -0.292785     1.167412      84.57
 H       5.250252     0.066066     2.114198      26.43
 H       6.317411     0.474854     0.579560      26.02
 H       6.662813    -0.992796     1.390671      25.43
 C       3.908862    -0.187560    -2.045648      16.50
 O       4.482157    -1.467449    -2.553490     126.43
 H       5.393478    -1.701760    -1.964201      22.70
 C       3.354403     0.795656    -2.935587      44.40
 H       3.308005     0.569825    -3.963210      21.99
 C       2.778889     2.174458    -0.840857      33.33
 C       1.946977     3.300898    -0.403212      76.06
 H       1.755474     4.226089    -1.166688      17.18
 O       2.346030     3.771703     0.943144     349.21
 H       3.155838     3.847491     1.422030      30.81
 C       0.183919     3.124299    -0.402482      54.13
 H       0.079394     2.703728    -1.443280      20.28
 C      -0.645573     4.416335     0.022804      98.57
 O      -0.147193     5.608249    -0.784690     269.48
 H      -0.257920     5.135141    -1.713049      24.55
 H      -0.698773     4.625992     1.093858      24.31
 H      -1.603437     4.174126    -0.339405      22.69
 C      -1.120180    -1.509168    -0.429314     -18.16
 H      -0.568830    -2.575352    -0.492102      18.41
 C      -3.078973    -0.124164    -0.652612      94.93
 H      -4.062084    -0.117899    -1.017730      23.82
 C      -2.354500     0.988593    -0.529545     -11.78
 O      -2.838922     2.426062    -0.515134     152.59
 C      -4.171358     2.421311    -0.743085     114.20
 H      -4.409282     1.989422     0.242905      24.05
 H      -4.512731     3.609103    -0.895924      23.58
 H      -4.335029     1.771023    -1.563597      24.57
 C      -0.888756     0.876974    -0.136915     -19.16
 O      -0.115395     2.006359     0.362460     142.04
 C      -0.335817    -0.372637    -0.157924      36.54
 H       0.541376    -0.606900     0.417806      23.10
 C      -2.508527    -1.302377    -0.633613      33.03
 C      -3.147172    -2.660307    -0.959959      55.15
 H      -3.851063    -2.376496    -2.017335      22.03
 O      -2.171182    -3.560621    -1.650626     145.13
 H      -2.587835    -4.558217    -1.588931      18.22
 C      -3.756408    -3.303812     0.470644      93.84
 H      -2.782230    -3.410963     0.839283      26.66
 O      -4.374360    -2.156379     1.003353     311.89
 H      -4.303687    -2.351183     2.081081      24.78
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 C      -4.535917    -4.593868     0.317084      97.69
 O      -3.869100    -5.545495    -0.544530     378.14
 H      -3.201571    -5.964743    -0.072645      33.44
 H      -5.573093    -4.337328    -0.060711      26.03
 H      -4.908442    -4.906647     1.353003      27.45
55
name = lig-etoh-frame_934
 C       2.707425     1.914567    -2.306851      66.28
 H       2.295389     2.586128    -3.033573      23.73
 C       3.355675     1.176248     0.100379      44.37
 H       3.746244     1.360690     1.163234      21.28
 C       3.952903    -0.019973    -0.585258       5.42
 O       4.747745    -0.905037     0.130678     228.52
 C       5.690843    -0.310988     1.131914     105.36
 H       5.084625    -0.034762     1.976227      26.68
 H       6.241700     0.464475     0.556464      26.61
 H       6.460206    -0.944904     1.540859      26.53
 C       3.870010    -0.187660    -1.996953      15.85
 O       4.469122    -1.487346    -2.584757     177.18
 H       5.207365    -1.724879    -1.900172      23.62
 C       3.378319     0.735301    -2.915479      35.26
 H       3.227742     0.739184    -4.066883      21.51
 C       2.799421     2.105345    -0.888579      18.54
 C       1.916989     3.338712    -0.342970      85.54
 H       1.898176     4.063541    -1.076301      21.35
 O       2.292550     3.777741     0.944475     353.36
 H       3.172998     3.795799     1.401522      28.00
 C       0.196972     3.127505    -0.352851      66.23
 H       0.058827     2.802686    -1.396551      19.88
 C      -0.662500     4.413566    -0.011595      90.27
 O      -0.137700     5.576279    -0.763632     290.61
 H      -0.112405     5.508960    -1.800006      25.41
 H      -0.613763     4.749688     1.053948      23.01
 H      -1.772856     4.248496    -0.248233      21.46
 C      -1.056578    -1.557530    -0.434529      92.25
 H      -0.720047    -2.495138    -0.470998      26.72
 C      -3.122004    -0.158009    -0.694278      49.04
 H      -4.209678    -0.122562    -0.919494      23.53
 C      -2.273613     1.049742    -0.455207     -20.27
 O      -2.745659     2.377683    -0.540485     147.46
 C      -4.184465     2.437260    -0.636599     107.65
 H      -4.970372     1.778388     0.087070      23.64
 H      -4.569721     3.275823    -1.126991      25.54
 H      -4.500905     1.846620    -1.801235      23.17
 C      -0.837251     0.930632    -0.202239       6.57
 O      -0.150529     2.019211     0.386451     171.23
 C      -0.369565    -0.329198    -0.157865      52.40
 H       0.687474    -0.478304     0.296482      22.39
 C      -2.424651    -1.374536    -0.604750      -0.27
 C      -3.156963    -2.604266    -1.020033      93.15
 H      -3.945735    -2.475546    -1.617388      22.67
 O      -2.174005    -3.548909    -1.667248     229.71
 H      -2.526820    -4.330035    -1.412198      21.23
 C      -3.746277    -3.329506     0.341730      71.62
 H      -2.819957    -3.344619     1.128794      18.63
 O      -4.421689    -2.133455     1.096712     301.37
 H      -4.484386    -2.244277     2.105518      27.66
 C      -4.592429    -4.594378     0.324815      91.27
 O      -3.896247    -5.536965    -0.523372     358.09
 H      -2.944065    -5.947789    -0.158354      23.35
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 H      -5.545382    -4.435635    -0.307300      24.86
 H      -4.911538    -4.948660     1.337822      27.49
55
name = lig-etoh-frame_935
 C       2.722175     1.965312    -2.295977      29.77
 H       2.264169     2.747515    -2.953692      19.01
 C       3.385702     1.102093     0.035686      82.49
 H       3.859680     1.676136     0.864944      23.91
 C       3.963349    -0.018819    -0.486198      17.86
 O       4.798341    -0.950445     0.180105     251.00
 C       5.631350    -0.320369     1.075637     103.90
 H       4.913329     0.104830     1.931642      23.35
 H       6.092552     0.614752     0.705540      26.03
 H       6.195801    -1.206224     1.533465      24.26
 C       3.874752    -0.273133    -1.988330      11.23
 O       4.439371    -1.458854    -2.587487     190.92
 H       4.997976    -1.777589    -1.908017      26.78
 C       3.346629     0.727591    -2.867546      37.69
 H       3.375495     0.640093    -3.908146      22.34
 C       2.753614     2.061726    -0.901887      62.05
 C       1.881584     3.354713    -0.284730     108.43
 H       2.257098     4.206185    -1.099780      21.29
 O       2.207309     3.790972     0.976838     288.75
 H       3.246851     3.785681     0.905475      26.65
 C       0.263821     3.153376    -0.353170      68.24
 H       0.005949     3.115573    -1.445318      17.98
 C      -0.657920     4.429210    -0.070890     100.34
 O      -0.134212     5.558305    -0.726216     322.09
 H       0.054231     5.615989    -1.682936      28.68
 H      -0.431295     4.745684     0.956599      23.51
 H      -1.734411     4.293581    -0.139030      23.41
 C      -1.006190    -1.522906    -0.422601      66.62
 H      -0.575027    -2.639566    -0.386856      20.51
 C      -3.110516    -0.115214    -0.721874       6.20
 H      -4.223097    -0.098159    -0.724707      22.33
 C      -2.211052     1.091897    -0.400938      -0.61
 O      -2.678551     2.313734    -0.550975     126.98
 C      -4.239695     2.395540    -0.598887     111.35
 H      -5.118881     1.972078    -0.220289      26.56
 H      -4.558812     3.431081    -0.993967      25.52
 H      -4.548552     1.838392    -1.680599      24.48
 C      -0.860120     1.019181    -0.251154      17.02
 O      -0.200539     1.991224     0.440595     175.23
 C      -0.312413    -0.358846    -0.133100      42.39
 H       0.729711    -0.270280    -0.006708      22.71
 C      -2.358334    -1.479903    -0.624031      -9.24
 C      -3.166966    -2.623080    -1.030097      87.21
 H      -4.341531    -2.450644    -1.500591      19.70
 O      -2.192863    -3.515183    -1.682602     159.89
 H      -2.579894    -4.459529    -1.278629      12.75
 C      -3.697626    -3.269155     0.294410      93.98
 H      -3.030218    -3.632697     1.023345      20.44
 O      -4.488512    -2.122967     1.157993     284.97
 H      -4.408191    -2.331568     2.095331      26.30
 C      -4.650955    -4.578991     0.292087      93.98
 O      -3.906016    -5.549299    -0.511523     354.98
 H      -3.078466    -5.952563    -0.081579      26.27
 H      -5.490607    -4.454941    -0.379458      25.80
 H      -4.822689    -5.000485     1.295996      29.58
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name = lig-etoh-frame_936
 C       2.767089     1.948386    -2.280242      37.13
 H       2.300928     2.782774    -2.784708      16.59
 C       3.418912     1.109372    -0.065735      74.89
 H       3.725960     1.703509     0.774164      20.24
 C       3.985844    -0.066429    -0.474738      17.60
 O       4.816429    -0.997944     0.176897     269.84
 C       5.566100    -0.313423     1.106118     121.05
 H       4.985663     0.131359     1.875606      27.74
 H       6.175348     0.588227     0.815461      27.19
 H       6.114662    -1.191450     1.489613      25.56
 C       3.875334    -0.346505    -1.974598       6.90
 O       4.397092    -1.398993    -2.576642     136.01
 H       4.922161    -2.042236    -1.791987      20.55
 C       3.299113     0.742118    -2.772826      59.51
 H       3.552848     0.446234    -3.869243      24.25
 C       2.655632     2.047872    -0.875802      54.38
 C       1.840184     3.362460    -0.305661     113.67
 H       2.265303     4.103742    -0.868762      23.92
 O       2.159972     3.797977     1.030826     313.44
 H       3.030260     4.032629     0.744805      29.44
 C       0.328229     3.208000    -0.403476      58.34
 H       0.054531     3.068876    -1.476625      18.78
 C      -0.593920     4.446769    -0.078087     100.75
 O      -0.130566     5.590249    -0.677959     313.00
 H       0.163625     5.330339    -1.727052      23.32
 H      -0.385844     4.623001     1.006307      22.61
 H      -1.678563     4.211288    -0.203200      22.00
 C      -0.935689    -1.516306    -0.393344      34.91
 H      -0.358240    -2.382079    -0.301057      24.33
 C      -2.977271    -0.101454    -0.705623      56.42
 H      -4.037298    -0.055105    -0.581262      24.62
 C      -2.245719     1.034817    -0.405502      13.03
 O      -2.708066     2.296065    -0.537270     123.36
 C      -4.278872     2.402629    -0.673655      90.36
 H      -5.097146     1.937157     0.208256      23.07
 H      -4.261329     3.521592    -0.505866      23.42
 H      -4.405251     1.798083    -1.673538      23.01
 C      -0.855297     0.986304    -0.248656       1.21
 O      -0.226355     1.998350     0.474436     110.10
 C      -0.231712    -0.326246    -0.128387      30.88
 H       0.929908    -0.245616    -0.230699      21.09
 C      -2.390206    -1.440696    -0.687527      -8.93
 C      -3.221443    -2.690867    -0.997884     106.05
 H      -3.990437    -2.391761    -1.562551      23.95
 O      -2.254984    -3.510975    -1.690078     230.64
 H      -2.469187    -4.465619    -1.523764      18.21
 C      -3.720778    -3.211255     0.344351      77.42
 H      -2.801329    -3.771353     0.893298      17.92
 O      -4.549561    -2.135694     1.165452     271.41
 H      -4.052061    -2.520803     2.131984      18.86
 C      -4.659462    -4.536326     0.213260      78.83
 O      -3.912623    -5.571470    -0.515572     342.90
 H      -3.287938    -6.075699     0.101615      28.32
 H      -5.732879    -4.372701    -0.306603      25.62
 H      -4.851200    -4.906099     1.286139      28.35
55
name = lig-etoh-frame_937
 C       2.790556     1.909703    -2.231507      56.86
 H       2.411020     2.707517    -2.900643      19.74
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 C       3.432320     1.190692    -0.136267      58.24
 H       3.516127     1.419203     1.027250      18.44
 C       4.000332    -0.152242    -0.582875      23.13
 O       4.799067    -1.024376     0.133946     262.80
 C       5.556876    -0.309719     1.199165     101.10
 H       4.866038     0.129577     2.075492      25.36
 H       6.295557     0.355896     0.712172      27.55
 H       6.295659    -1.002491     1.666770      26.64
 C       3.831972    -0.318375    -1.895789      26.12
 O       4.379255    -1.387946    -2.559908     235.87
 H       4.713552    -2.005795    -1.967748      27.28
 C       3.293568     0.697872    -2.705047      54.63
 H       3.514855     0.531428    -3.740808      27.05
 C       2.559780     2.040886    -0.843803      58.40
 C       1.809225     3.322384    -0.318020      97.41
 H       2.102372     4.257061    -1.049227      21.31
 O       2.133872     3.794234     1.079758     244.37
 H       2.960702     4.468252     1.123973      26.30
 C       0.337384     3.246171    -0.481298      65.48
 H       0.169502     2.778813    -1.479191      20.17
 C      -0.501095     4.430915    -0.009106     105.75
 O      -0.109550     5.650876    -0.669920     332.64
 H       0.067026     5.372808    -1.520033      31.59
 H      -0.514684     4.486796     1.086027      23.68
 H      -1.513130     4.104524    -0.375109      21.37
 C      -0.907156    -1.481581    -0.369550     -59.77
 H      -0.206742    -2.400870    -0.293371      20.40
 C      -2.852066    -0.156802    -0.673331      99.74
 H      -3.982965    -0.036792    -0.591843      22.58
 C      -2.254776     0.987113    -0.444943      12.42
 O      -2.805987     2.293037    -0.502442     155.99
 C      -4.288147     2.422123    -0.693109     116.68
 H      -4.405920     2.028491     0.262456      24.99
 H      -4.249191     3.473574    -0.389469      24.61
 H      -4.521697     1.923455    -1.823231      21.44
 C      -0.822226     0.890672    -0.182552      -7.50
 O      -0.225871     2.053091     0.458448      89.45
 C      -0.137266    -0.258457    -0.173282      67.65
 H       0.888236    -0.381357    -0.165441      23.71
 C      -2.375573    -1.358045    -0.741823     -13.23
 C      -3.233114    -2.717320    -0.936873      68.25
 H      -3.951537    -2.328294    -1.917383      22.05
 O      -2.321613    -3.531127    -1.707665     247.47
 H      -2.502858    -4.456662    -1.721650      23.16
 C      -3.792839    -3.211858     0.426650      99.07
 H      -2.770681    -3.418140     0.719033      23.72
 O      -4.546188    -2.208731     1.167875     369.94
 H      -4.137065    -2.216927     2.006830      30.39
 C      -4.662025    -4.478195     0.146503     104.77
 O      -3.926648    -5.583033    -0.530001     292.87
 H      -3.584300    -6.277207     0.247263      25.39
 H      -5.629515    -4.289366    -0.200219      28.19
 H      -4.944787    -4.746038     1.154464      27.82
55
name = lig-etoh-frame_938
 C       2.770515     1.867124    -2.200386      50.04
 H       2.574862     2.511990    -3.062998      21.24
 C       3.434196     1.220460    -0.105472      82.28
 H       3.309649     1.088251     0.909467      22.15
 C       3.988086    -0.126886    -0.610726      23.46
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 O       4.786020    -1.035622     0.112363     235.24
 C       5.569330    -0.321630     1.304188      89.47
 H       4.925406     0.094366     1.955654      29.78
 H       6.175036     0.337757     0.624517      26.63
 H       6.305906    -0.983084     1.870765      26.35
 C       3.786639    -0.305641    -1.887709      29.18
 O       4.358323    -1.393554    -2.573640     217.74
 H       4.695069    -2.070892    -1.904694      24.39
 C       3.294800     0.666666    -2.673380      39.67
 H       3.385901     0.654088    -3.780254      24.08
 C       2.518575     2.051920    -0.809543      85.88
 C       1.845998     3.328231    -0.318166      97.77
 H       1.895125     4.065890    -1.058794      23.32
 O       2.120674     3.785653     1.110046     296.88
 H       2.619416     4.575263     1.401108      29.47
 C       0.319028     3.212630    -0.525838      62.48
 H       0.165517     2.726697    -1.528468      20.29
 C      -0.433742     4.396958     0.028476      99.80
 O      -0.087564     5.723740    -0.625501     249.21
 H       0.029517     5.585911    -1.746889      23.97
 H      -0.545804     4.453973     1.126351      23.84
 H      -1.399463     4.148672    -0.380840      22.36
 C      -0.893540    -1.429588    -0.373200      35.05
 H      -0.424995    -2.438838    -0.400005      18.59
 C      -2.892972    -0.179535    -0.652552      39.28
 H      -3.928477    -0.150401    -0.809265      21.15
 C      -2.167089     1.034785    -0.476149      11.31
 O      -2.870900     2.272096    -0.479328     185.69
 C      -4.219114     2.437435    -0.679462     115.99
 H      -4.473507     1.780692     0.269393      22.07
 H      -4.580976     3.563876    -0.661676      23.63
 H      -4.950013     2.290391    -1.612123      23.01
 C      -0.813588     0.911673    -0.082174      13.86
 O      -0.216225     2.118767     0.404348     127.72
 C      -0.073098    -0.283036    -0.241375      34.19
 H       1.039381    -0.399904     0.083246      19.58
 C      -2.235961    -1.431370    -0.753941      33.79
 C      -3.242168    -2.636464    -0.960999      75.93
 H      -3.979565    -2.457106    -1.609982      26.24
 O      -2.365683    -3.560929    -1.720127     197.78
 H      -2.791571    -4.577311    -1.766007      20.02
 C      -3.851717    -3.216658     0.441717      86.96
 H      -2.841996    -3.292687     1.030083      22.41
 O      -4.533072    -2.292742     1.146244     361.45
 H      -4.241946    -1.932594     2.117115      27.29
 C      -4.637851    -4.442931     0.139751      81.83
 O      -3.965135    -5.584285    -0.532643     303.21
 H      -3.763644    -6.219184     0.063344      31.36
 H      -5.634252    -4.092407    -0.527494      24.60
 H      -5.066496    -4.802488     1.172519      25.19
55
name = lig-etoh-frame_939
 C       2.721262     1.827486    -2.195793      46.96
 H       2.543492     2.522134    -3.018314      23.03
 C       3.407923     1.163701    -0.034749      86.24
 H       3.175579     1.037177     1.116761      18.19
 C       3.974002    -0.005258    -0.513434      28.69
 O       4.776808    -1.030415     0.126914     221.77
 C       5.598593    -0.355578     1.335249      93.26
 H       4.773864     0.268425     1.992196      25.22
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 H       6.049055     0.500681     0.842074      28.34
 H       6.108540    -1.123762     1.868257      26.74
 C       3.783059    -0.376813    -1.971876      16.60
 O       4.333823    -1.416994    -2.595740     163.77
 H       4.760149    -2.051161    -1.771859      22.14
 C       3.270102     0.691791    -2.705143      51.44
 H       3.274619     0.614665    -3.839001      20.70
 C       2.568007     2.071854    -0.786277      81.13
 C       1.879512     3.350791    -0.287510     108.34
 H       2.117725     4.172320    -1.118460      21.30
 O       2.083390     3.743946     1.122230     315.97
 H       2.477542     4.607222     1.204122      29.91
 C       0.321613     3.125276    -0.515681      81.76
 H       0.053349     3.012158    -1.591372      21.24
 C      -0.413805     4.397642    -0.013384      86.07
 O      -0.056503     5.783131    -0.582998     273.15
 H      -0.030747     5.789250    -1.520343      30.61
 H      -0.325005     4.501768     1.078426      23.93
 H      -1.541463     4.294882    -0.241769      22.59
 C      -0.847638    -1.432582    -0.412805      60.88
 H      -0.506913    -2.472190    -0.450182      20.13
 C      -2.935832    -0.175409    -0.657328       7.54
 H      -4.005032    -0.217429    -1.082568      18.57
 C      -2.132191     1.058346    -0.499416       2.57
 O      -2.850987     2.264761    -0.484109     191.48
 C      -4.232639     2.452255    -0.586494     126.40
 H      -5.083342     1.867144    -0.113118      24.02
 H      -4.535386     3.438771    -0.634948      26.90
 H      -5.017023     2.154596    -1.671981      22.18
 C      -0.784423     1.009887    -0.006438       3.61
 O      -0.202471     2.167853     0.351745     187.59
 C      -0.030918    -0.321025    -0.268816      23.63
 H       0.906478    -0.299734     0.211770      20.49
 C      -2.162755    -1.494173    -0.736320      24.76
 C      -3.183240    -2.563940    -0.972512      56.41
 H      -4.328124    -2.294276    -1.472631      21.55
 O      -2.415695    -3.620620    -1.731554     230.94
 H      -2.997399    -4.348972    -1.630919      22.02
 C      -3.770598    -3.216276     0.433766      92.21
 H      -3.110205    -3.598638     1.240725      21.71
 O      -4.583555    -2.320134     1.131706     350.76
 H      -4.131814    -2.107553     2.032108      26.87
 C      -4.672423    -4.449394     0.147339     103.51
 O      -4.025310    -5.549437    -0.554264     302.57
 H      -3.703549    -6.296230     0.094294      27.35
 H      -5.287938    -4.105035    -0.620516      28.45
 H      -5.152421    -4.830837     0.989127      28.27
55
name = lig-etoh-frame_940
 C       2.650601     1.836126    -2.175052      46.95
 H       2.290624     2.698704    -2.785158      25.51
 C       3.319585     1.100143     0.100870      49.50
 H       3.317917     1.326224     1.120386      23.74
 C       3.978975     0.043012    -0.497795      16.38
 O       4.770842    -0.981194     0.177984     228.31
 C       5.548775    -0.360525     1.327389     103.15
 H       4.880426     0.038516     1.977793      28.64
 H       6.255770     0.528140     1.121581      26.27
 H       5.999628    -1.309903     1.814366      24.91
 C       3.791623    -0.376387    -1.986676      14.51
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 O       4.328543    -1.484302    -2.599033     247.91
 H       4.782392    -1.867865    -1.950988      30.16
 C       3.245109     0.677513    -2.788329      52.44
 H       3.224651     0.529057    -3.827568      20.48
 C       2.685608     2.078392    -0.781516      34.14
 C       1.895343     3.369891    -0.283848     111.66
 H       2.395180     4.178692    -0.793460      21.53
 O       2.042844     3.686357     1.112565     310.86
 H       2.473626     4.595803     0.883750      24.96
 C       0.346567     3.121251    -0.521719      91.58
 H       0.017768     3.161642    -1.587873      21.49
 C      -0.437770     4.459266    -0.075778      90.95
 O      -0.022190     5.822685    -0.510166     266.11
 H      -0.034774     5.798838    -1.549866      27.60
 H      -0.038891     4.558219     0.957779      22.70
 H      -1.489096     4.369937    -0.068792      25.04
 C      -0.766948    -1.505342    -0.470960      28.21
 H      -0.224113    -2.542758    -0.398370      18.25
 C      -2.897551    -0.185338    -0.699034      58.61
 H      -3.850833    -0.110344    -1.157432      20.67
 C      -2.182780     1.022989    -0.495797      -8.62
 O      -2.809382     2.272230    -0.487840     113.16
 C      -4.358291     2.420306    -0.561288     101.06
 H      -5.255848     1.996431    -0.068687      24.61
 H      -4.285326     3.651002    -0.402837      23.01
 H      -4.244551     2.055537    -1.543471      23.17
 C      -0.759811     1.030525    -0.019875       9.25
 O      -0.179220     2.194954     0.339100     215.93
 C      -0.055018    -0.264439    -0.229921      -7.77
 H       0.994006    -0.335573     0.189496      19.65
 C      -2.235307    -1.416015    -0.712220      21.88
 C      -3.114378    -2.570812    -0.957419      86.31
 H      -3.938500    -2.108417    -1.300203      26.85
 O      -2.487865    -3.656023    -1.738225     231.63
 H      -3.128383    -4.447468    -1.527102      17.10
 C      -3.660297    -3.256352     0.442011      83.67
 H      -2.970749    -3.819426     1.111719      22.16
 O      -4.649856    -2.314812     1.126644     346.57
 H      -4.139827    -2.324787     1.922530      28.03
 C      -4.692433    -4.459316     0.122920      78.06
 O      -4.083855    -5.532192    -0.577734     276.59
 H      -3.445954    -6.153010     0.042371      25.58
 H      -5.381669    -4.028794    -0.797071      24.52
 H      -5.419623    -4.795274     1.013818      25.91
55
name = lig-etoh-frame_941
 C       2.598038     1.856891    -2.152962      45.35
 H       2.032570     2.673574    -2.597220      23.69
 C       3.218217     1.083133     0.201526      62.80
 H       3.545199     1.584568     1.221827      23.26
 C       3.995506    -0.007084    -0.545202      -1.04
 O       4.769731    -0.885740     0.233339     223.75
 C       5.500523    -0.396378     1.311943     118.66
 H       4.741030    -0.112687     2.227883      24.39
 H       6.383000     0.220975     1.209867      26.87
 H       5.975645    -1.255756     1.681529      26.72
 C       3.796202    -0.281522    -1.951338       5.46
 O       4.317420    -1.544639    -2.598544     164.90
 H       5.074502    -1.954903    -1.905425      22.75
 C       3.208516     0.649569    -2.838755      24.50
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 H       3.153129     0.453303    -4.003024      19.78
 C       2.793538     2.070031    -0.766273      41.16
 C       1.916174     3.325353    -0.293649     129.18
 H       2.420547     4.247601    -0.754365      22.57
 O       2.017570     3.642828     1.090597     315.30
 H       2.559978     4.476040     1.105744      27.28
 C       0.369819     3.247931    -0.586325      68.98
 H       0.136117     2.879707    -1.607374      21.32
 C      -0.417995     4.553828    -0.079910      89.61
 O       0.010070     5.846757    -0.466153     265.10
 H       0.039240     5.822794    -1.545126      26.09
 H      -0.014235     4.523030     0.936326      22.11
 H      -1.562020     4.342140    -0.003490      22.47
 C      -0.721556    -1.543311    -0.519713      19.71
 H      -0.098940    -2.371057    -0.388301      25.50
 C      -2.825811    -0.158985    -0.763253      79.77
 H      -3.866907    -0.029550    -1.120345      24.56
 C      -2.212085     1.000751    -0.442360      12.14
 O      -2.764336     2.267228    -0.455574     105.93
 C      -4.436529     2.439291    -0.580383      99.17
 H      -5.012711     1.933134     0.287936      23.87
 H      -4.315490     3.388293    -0.360321      27.26
 H      -4.054597     2.169989    -1.690409      19.41
 C      -0.786634     0.967117    -0.116828      10.29
 O      -0.152617     2.196858     0.363373     147.29
 C      -0.101396    -0.201557    -0.145816      24.83
 H       0.988305    -0.334596    -0.076375      21.00
 C      -2.232912    -1.352572    -0.678842     -10.49
 C      -3.029143    -2.645749    -0.882805      66.67
 H      -3.980629    -2.048075    -1.488924      18.95
 O      -2.577150    -3.673670    -1.745149     206.37
 H      -3.019511    -4.600856    -1.497288      14.93
 C      -3.629622    -3.321414     0.433081      85.23
 H      -2.631966    -3.664921     0.938245      19.82
 O      -4.667261    -2.320119     1.116657     236.59
 H      -4.308755    -2.384187     2.205136      21.06
 C      -4.738030    -4.427307     0.058239     100.42
 O      -4.115299    -5.553586    -0.599286     366.94
 H      -3.391792    -5.855056    -0.134702      34.91
 H      -5.446158    -4.031804    -0.564149      28.67
 H      -5.351378    -4.619844     0.863348      28.67
55
name = lig-etoh-frame_942
 C       2.594469     1.826457    -2.151289      47.84
 H       1.895268     2.503075    -2.684755      21.90
 C       3.196611     1.085788     0.215553      71.21
 H       3.640528     1.479750     1.101216      27.04
 C       3.973109    -0.026991    -0.535445       8.32
 O       4.762468    -0.795376     0.234452     222.96
 C       5.448160    -0.450805     1.374216     110.91
 H       4.897531    -0.142989     2.204073      27.96
 H       6.331648     0.212933     1.080535      24.77
 H       6.005071    -1.446472     1.661393      24.10
 C       3.829833    -0.222738    -1.932744      -1.50
 O       4.307601    -1.572459    -2.554593     173.27
 H       5.183910    -1.891164    -2.085448      24.64
 C       3.133799     0.668760    -2.845477       4.85
 H       3.077709     0.438001    -3.832937      22.47
 C       2.815867     2.062211    -0.732295      56.25
 C       1.965124     3.296332    -0.317776     123.12
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 H       2.222371     4.173791    -0.973468      24.81
 O       2.009899     3.604649     1.089943     336.67
 H       2.650934     4.211079     1.442356      29.74
 C       0.378357     3.368686    -0.663250      39.80
 H       0.280940     2.715069    -1.553127      19.72
 C      -0.381823     4.609009    -0.033012      97.50
 O       0.043135     5.881759    -0.469845     313.19
 H       0.138939     5.899696    -1.371408      33.51
 H      -0.197366     4.479569     1.059488      22.98
 H      -1.413096     4.408550    -0.154755      23.82
 C      -0.749358    -1.443791    -0.526373      54.92
 H      -0.068149    -2.422164    -0.409864      22.14
 C      -2.812950    -0.104207    -0.841138      44.59
 H      -3.921654    -0.133298    -0.972332      22.77
 C      -2.183826     1.040076    -0.368426      15.10
 O      -2.733665     2.260407    -0.396895      89.04
 C      -4.412350     2.422929    -0.607529      77.35
 H      -4.595220     1.758850     0.198270      23.55
 H      -4.553414     3.641664    -0.356276      22.81
 H      -4.844047     2.329910    -1.718331      22.89
 C      -0.825996     0.963793    -0.209877       1.22
 O      -0.136319     2.176940     0.380126      56.29
 C      -0.129837    -0.247197    -0.102440      47.26
 H       0.946262    -0.103300    -0.194132      21.24
 C      -2.098528    -1.437648    -0.653730       2.12
 C      -3.056118    -2.680772    -0.826432      94.33
 H      -3.837181    -2.447700    -1.411983      21.84
 O      -2.631420    -3.697793    -1.762327     269.59
 H      -2.967522    -4.506476    -1.503788      22.69
 C      -3.657380    -3.348864     0.400608      95.29
 H      -2.749966    -3.492019     0.974298      20.98
 O      -4.618649    -2.349011     1.138051     298.86
 H      -4.579289    -2.378417     2.030821      28.71
 C      -4.725355    -4.377505     0.004434      73.79
 O      -4.158241    -5.589613    -0.637771     284.50
 H      -3.212231    -5.728806    -0.070397      26.43
 H      -5.610485    -3.857960    -0.670435      24.63
 H      -5.224168    -4.678432     1.064711      25.52
55
name = lig-etoh-frame_943
 C       2.608398     1.770987    -2.158720      59.55
 H       1.969674     2.336843    -2.827262      22.16
 C       3.265793     1.078679     0.123900      39.09
 H       3.576723     1.277793     1.201163      21.51
 C       3.903233     0.030264    -0.474801      32.99
 O       4.746811    -0.762280     0.190040     227.48
 C       5.473912    -0.519270     1.448891     105.35
 H       4.855893    -0.013210     2.349220      24.63
 H       6.087800     0.312523     1.120812      25.62
 H       5.868401    -1.461591     1.672414      25.85
 C       3.878087    -0.234929    -1.948953      24.67
 O       4.295187    -1.546534    -2.491944     224.31
 H       5.119643    -1.747626    -2.173506      27.88
 C       3.072096     0.689879    -2.752816      45.23
 H       2.932285     0.412862    -3.886597      23.72
 C       2.734955     2.068014    -0.726977     100.33
 C       2.002283     3.323119    -0.338682     114.25
 H       2.293462     4.136447    -1.080196      23.29
 O       2.001712     3.565450     1.095285     294.97
 H       2.912656     3.886513     1.533910      25.45
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 C       0.414225     3.391933    -0.664584      34.23
 H       0.177071     3.024978    -1.683104      19.25
 C      -0.337509     4.616641     0.001863      83.56
 O       0.082026     5.939582    -0.460619     223.83
 H       0.257600     5.882839    -1.566383      25.26
 H      -0.337396     4.548565     1.100920      22.44
 H      -1.424745     4.514759    -0.419436      20.01
 C      -0.731764    -1.377881    -0.480348      74.50
 H      -0.308492    -2.290419    -0.501360      23.66
 C      -2.800509    -0.134581    -0.877480      22.20
 H      -3.852886    -0.243301    -0.868532      22.62
 C      -2.191705     1.072303    -0.351207      -0.40
 O      -2.757480     2.305855    -0.348846      95.87
 C      -4.327052     2.448779    -0.617634      92.49
 H      -4.601876     1.555518     0.033382      23.20
 H      -4.690360     3.343129    -0.358007      26.65
 H      -5.296879     2.242540    -1.518624      21.99
 C      -0.785415     1.023091    -0.222067      -2.95
 O      -0.138814     2.141892     0.361542      67.68
 C      -0.127280    -0.265095    -0.117648      55.76
 H       0.948797     0.018790    -0.080499      19.52
 C      -2.066580    -1.517437    -0.674053      -9.55
 C      -3.099322    -2.687437    -0.805522      62.91
 H      -4.136526    -2.285047    -1.370608      19.05
 O      -2.628247    -3.718549    -1.795412     197.26
 H      -3.092577    -4.671876    -1.478934      13.47
 C      -3.720824    -3.309731     0.396383      98.70
 H      -3.037460    -3.698415     1.289130      17.81
 O      -4.556709    -2.375189     1.098916     284.79
 H      -4.457690    -2.546391     2.188009      21.84
 C      -4.722984    -4.356305    -0.003226     111.64
 O      -4.183614    -5.615748    -0.667867     331.89
 H      -3.426592    -5.874242    -0.100808      30.52
 H      -5.376477    -3.971179    -0.637872      30.64
 H      -5.032651    -4.728073     0.884367      30.51
55
name = lig-etoh-frame_944
 C       2.585399     1.782329    -2.122048      33.45
 H       2.078434     2.419099    -2.868036      18.58
 C       3.351407     1.146270     0.044656      78.67
 H       3.219313     1.075149     1.163050      19.12
 C       3.869087     0.056326    -0.489945      33.20
 O       4.744089    -0.789949     0.160754     213.54
 C       5.466541    -0.529823     1.505538      93.03
 H       4.765483    -0.165697     2.264568      28.82
 H       6.175798     0.349300     1.346118      26.07
 H       5.905889    -1.537341     1.785131      25.94
 C       3.890952    -0.264223    -1.950307      33.01
 O       4.262995    -1.473816    -2.422964     162.84
 H       5.326725    -1.652971    -2.075532      21.90
 C       3.087212     0.584480    -2.675426      49.86
 H       2.798772     0.490193    -3.686297      27.17
 C       2.607810     2.065361    -0.776408      94.47
 C       1.997969     3.377281    -0.347456     115.68
 H       2.598515     4.194339    -0.888917      22.88
 O       2.019243     3.542401     1.100952     319.75
 H       2.980750     3.503166     1.235033      30.20
 C       0.462730     3.357773    -0.597289      43.02
 H       0.049073     3.505642    -1.660143      17.43
 C      -0.329117     4.614140    -0.022881      91.31
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 O       0.139842     5.998708    -0.473411     253.78
 H       0.277444     5.808478    -1.398471      32.13
 H      -0.369431     4.669831     1.059316      24.50
 H      -1.284973     4.556020    -0.455961      23.63
 C      -0.721283    -1.425051    -0.424949      19.89
 H      -0.147815    -2.474763    -0.494131      20.04
 C      -2.754623    -0.221978    -0.844837      41.23
 H      -3.909497    -0.263645    -0.887435      23.98
 C      -2.215650     1.055732    -0.411605     -22.82
 O      -2.831931     2.388760    -0.331775     164.77
 C      -4.257036     2.394529    -0.601818     122.04
 H      -4.815510     1.634861     0.024694      25.43
 H      -4.640481     3.414715    -0.061432      24.05
 H      -4.845786     2.099810    -1.416261      26.12
 C      -0.730155     1.077905    -0.170619       3.11
 O      -0.135932     2.127168     0.308022     107.74
 C      -0.074686    -0.140881    -0.156703      51.86
 H       0.980830    -0.226970     0.115517      20.17
 C      -2.176830    -1.491865    -0.734255      -8.38
 C      -3.143939    -2.676893    -0.865840      71.29
 H      -3.931398    -2.049882    -1.091744      22.13
 O      -2.617808    -3.745679    -1.809700     239.42
 H      -3.115243    -4.525123    -1.645355      20.67
 C      -3.760565    -3.288303     0.451250     102.27
 H      -3.208699    -3.930312     1.087017      19.32
 O      -4.515173    -2.374446     1.075277     385.77
 H      -4.071648    -2.611660     1.956124      21.31
 C      -4.688986    -4.404140    -0.002566      77.30
 O      -4.203970    -5.629264    -0.699753     296.79
 H      -3.597039    -6.168375    -0.092663      28.56
 H      -5.524067    -3.995751    -0.822217      24.88
 H      -5.269923    -4.820898     0.976175      27.04
55
name = lig-etoh-frame_945
 C       2.542331     1.799215    -2.117475      41.77
 H       2.176394     2.568657    -2.799754      19.59
 C       3.365692     1.273350     0.013891     100.57
 H       3.048815     1.171455     1.019950      20.06
 C       3.931229     0.018997    -0.561017      13.07
 O       4.765317    -0.848960     0.166276     218.12
 C       5.432186    -0.521530     1.514075      98.20
 H       4.570922    -0.351160     2.274329      26.51
 H       6.274408     0.161938     1.561381      26.43
 H       5.940856    -1.449468     1.821347      26.63
 C       3.856028    -0.274718    -1.891783      38.48
 O       4.280530    -1.420959    -2.358541     244.67
 H       5.141010    -1.624344    -1.987376      25.64
 C       3.094904     0.500879    -2.629753      48.09
 H       2.812692     0.349721    -3.690654      24.92
 C       2.504674     2.059410    -0.818067      87.20
 C       1.966207     3.420775    -0.328763     119.41
 H       2.615966     4.255834    -0.653021      22.31
 O       2.070173     3.523430     1.090936     372.00
 H       3.000361     3.288070     1.175366      28.68
 C       0.475839     3.363768    -0.519367      76.95
 H       0.159454     3.475528    -1.545862      19.41
 C      -0.313838     4.640911    -0.044857      83.39
 O       0.203046     6.023467    -0.479515     234.81
 H       0.350957     5.904939    -1.489703      29.55
 H      -0.361868     4.754862     1.072766      24.69
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 H      -1.394584     4.493750    -0.426530      22.85
 C      -0.749132    -1.496203    -0.383685     -21.00
 H      -0.055665    -2.270188    -0.306984      15.35
 C      -2.773138    -0.239181    -0.772196      56.48
 H      -3.777699    -0.177105    -1.007223      22.09
 C      -2.182293     1.035869    -0.498684     -12.49
 O      -2.900068     2.420803    -0.341754      94.67
 C      -4.225933     2.351166    -0.490459      88.68
 H      -4.792015     1.715327     0.229423      23.90
 H      -4.436378     3.335617    -0.102922      24.03
 H      -4.311650     2.096196    -1.975961      18.95
 C      -0.773005     1.087532    -0.140451      16.04
 O      -0.090895     2.199281     0.253241     153.84
 C      -0.015603    -0.095546    -0.209658     -17.71
 H       0.955418    -0.376581     0.212584      18.54
 C      -2.201023    -1.459729    -0.778141      28.17
 C      -3.137726    -2.680970    -0.921324      68.08
 H      -4.105136    -2.046629    -1.290053      23.42
 O      -2.608319    -3.725499    -1.816994     218.38
 H      -3.223788    -4.553663    -1.731654      19.05
 C      -3.756554    -3.350762     0.420303      82.74
 H      -2.866218    -3.971719     0.940230      22.34
 O      -4.478895    -2.339312     1.100919     346.29
 H      -4.053795    -2.262091     2.044414      26.74
 C      -4.746892    -4.502862    -0.014852     109.52
 O      -4.205820    -5.631020    -0.727355     259.81
 H      -3.870624    -6.476110    -0.104321      25.89
 H      -5.431047    -4.131890    -0.657686      30.01
 H      -5.403778    -4.687534     0.757104      29.05
55
name = lig-etoh-frame_946
 C       2.504954     1.759998    -2.207742      50.19
 H       2.177951     2.571100    -2.863642      17.15
 C       3.355485     1.323756    -0.031488     109.65
 H       3.153884     1.445661     1.138020      15.07
 C       4.026407     0.062425    -0.514834      25.13
 O       4.811655    -0.904946     0.191459     255.47
 C       5.368344    -0.536882     1.506383     109.45
 H       4.500966    -0.440866     2.253446      27.28
 H       6.176110     0.240498     1.573536      27.61
 H       5.852228    -1.493206     1.764164      26.30
 C       3.803440    -0.288950    -1.807300      17.27
 O       4.327997    -1.432372    -2.329277     221.05
 H       5.100312    -1.715209    -1.781393      25.52
 C       3.015229     0.557368    -2.654700      48.94
 H       3.029057     0.071600    -3.707460      23.98
 C       2.467578     2.081544    -0.805944      92.36
 C       1.933053     3.424793    -0.279523     103.98
 H       2.395537     4.392241    -0.771916      19.20
 O       2.141582     3.504393     1.094601     360.01
 H       3.087432     3.212914     1.422652      27.55
 C       0.439915     3.426464    -0.474255      77.19
 H       0.338336     3.057714    -1.598665      18.12
 C      -0.317046     4.705399    -0.043682      98.09
 O       0.262923     6.003937    -0.495036     238.72
 H       0.384443     6.112096    -1.563838      26.45
 H      -0.296385     4.771701     1.025002      26.09
 H      -1.341626     4.514789    -0.328624      24.53
 C      -0.792489    -1.453497    -0.360889      32.64
 H      -0.072110    -2.329799    -0.133706      16.40
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 C      -2.829166    -0.152389    -0.704234      24.41
 H      -3.884493    -0.090855    -1.156108      19.02
 C      -2.128570     1.056225    -0.559944       5.46
 O      -2.867627     2.372874    -0.341203     158.37
 C      -4.248779     2.315099    -0.471241     120.37
 H      -4.752047     1.559649     0.234474      23.90
 H      -4.592326     3.484708    -0.362161      23.92
 H      -4.118479     2.296624    -1.399856      25.32
 C      -0.816544     1.079733    -0.155116     -10.26
 O      -0.035942     2.307915     0.219498     131.62
 C      -0.032421    -0.188750    -0.253290       4.74
 H       1.004912    -0.167689     0.151468      17.67
 C      -2.118326    -1.498866    -0.778524      24.69
 C      -3.163992    -2.678010    -0.976758      76.32
 H      -4.015204    -2.533587    -1.608589      23.42
 O      -2.598544    -3.684334    -1.823808     237.10
 H      -3.216793    -4.522540    -1.758339      22.24
 C      -3.699056    -3.448570     0.347281      75.11
 H      -2.787971    -3.632722     0.836747      25.14
 O      -4.433765    -2.307591     1.147754     318.49
 H      -4.192392    -1.915583     2.100176      27.05
 C      -4.810539    -4.581615    -0.023343      77.69
 O      -4.203497    -5.660637    -0.747580     297.01
 H      -4.099704    -6.355957    -0.202535      31.32
 H      -5.552562    -4.032387    -0.854644      24.77
 H      -5.524259    -4.802337     0.905116      25.19
55
name = lig-etoh-frame_947
 C       2.444886     1.749369    -2.294930      44.73
 H       2.047270     2.429482    -3.068961      21.11
 C       3.344464     1.304781    -0.020690      57.72
 H       3.545850     1.639526     0.942410      20.42
 C       4.102820     0.159612    -0.401679      40.65
 O       4.858095    -0.923727     0.218827     272.51
 C       5.304795    -0.586351     1.499511     112.69
 H       4.484494    -0.364300     2.244728      25.55
 H       5.838932     0.379315     1.442556      26.09
 H       5.817794    -1.553363     1.791679      23.35
 C       3.731036    -0.288095    -1.753604      17.89
 O       4.391819    -1.463550    -2.321721     155.49
 H       4.963958    -1.873232    -1.429914      21.38
 C       2.967445     0.574402    -2.708923      48.03
 H       3.094277     0.185569    -3.654382      22.40
 C       2.503670     2.108813    -0.830619      71.14
 C       1.928612     3.425831    -0.237812     116.74
 H       2.173218     4.266892    -0.932412      20.86
 O       2.215263     3.494739     1.138162     387.36
 H       3.111911     3.368004     1.450729      29.98
 C       0.394658     3.487502    -0.520075      80.55
 H       0.423021     3.054342    -1.479383      20.50
 C      -0.313494     4.782134    -0.057417      99.54
 O       0.317749     5.981012    -0.521473     289.64
 H       0.288957     5.979472    -1.427690      33.01
 H      -0.172746     4.794027     1.077289      24.21
 H      -1.412341     4.696594    -0.327486      23.28
 C      -0.773610    -1.402019    -0.342167      70.00
 H      -0.403854    -2.402517    -0.097285      17.67
 C      -2.865964    -0.105328    -0.691644      13.96
 H      -3.845603    -0.067381    -1.094929      19.49
 C      -2.144463     1.127594    -0.574165       7.22
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 O      -2.748982     2.291972    -0.311998     147.26
 C      -4.289561     2.328801    -0.420638      85.54
 H      -4.769168     1.513694     0.029477      24.32
 H      -4.789280     3.292163    -0.462611      23.74
 H      -4.647763     2.094273    -1.871976      20.29
 C      -0.742685     1.073400    -0.202629     -19.94
 O      -0.030161     2.344718     0.239548     127.49
 C      -0.111936    -0.251532    -0.256269      52.33
 H       0.928895    -0.012957    -0.094176      18.25
 C      -2.121648    -1.481822    -0.752974      -0.94
 C      -3.191741    -2.705533    -1.024172      66.20
 H      -4.074816    -2.443141    -1.735252      21.15
 O      -2.554203    -3.668770    -1.848468     270.04
 H      -3.023048    -4.443926    -1.766266      27.49
 C      -3.668348    -3.460171     0.294986      68.05
 H      -2.705542    -3.615718     0.953309      20.83
 O      -4.406214    -2.283285     1.152348     311.81
 H      -4.012423    -2.203783     2.009834      27.35
 C      -4.880943    -4.594281    -0.034039      94.01
 O      -4.216534    -5.687871    -0.775032     273.10
 H      -4.120671    -6.469319    -0.106362      27.88
 H      -5.455257    -4.092784    -0.723620      28.61
 H      -5.315328    -4.992781     0.836288      26.73
55
name = lig-etoh-frame_948
 C       2.366503     1.786718    -2.318964      43.39
 H       1.842857     2.292771    -3.126818      21.68
 C       3.355202     1.282128     0.026652      98.05
 H       3.909019     1.875280     0.903404      24.97
 C       4.122375     0.194317    -0.390780      21.21
 O       4.871858    -0.896932     0.221664     240.72
 C       5.258465    -0.633384     1.528597     112.73
 H       4.354756    -0.367542     2.238411      25.24
 H       5.731721     0.373443     1.424764      25.12
 H       5.906678    -1.368842     1.950273      25.21
 C       3.689061    -0.278441    -1.728992      17.17
 O       4.446374    -1.475240    -2.271725     209.43
 H       4.659839    -1.879065    -1.518022      28.94
 C       2.991262     0.507875    -2.713564      31.83
 H       3.010212     0.381054    -3.926146      19.12
 C       2.572197     2.124976    -0.916485      49.89
 C       1.942550     3.417694    -0.228450     129.66
 H       2.339867     4.255057    -0.945079      19.87
 O       2.265253     3.509730     1.189888     339.74
 H       3.241180     3.660722     1.228139      29.79
 C       0.385560     3.502946    -0.562058      52.95
 H       0.242804     3.414238    -1.741687      16.87
 C      -0.315209     4.837731    -0.056770     102.70
 O       0.371222     5.969251    -0.543031     244.20
 H       0.214431     5.801727    -1.621083      25.97
 H      -0.153628     4.822071     0.993262      24.63
 H      -1.394890     4.956663    -0.287115      23.33
 C      -0.811658    -1.452519    -0.343201      46.26
 H      -0.426386    -2.448904    -0.138768      19.80
 C      -2.836553    -0.120487    -0.727867      50.75
 H      -3.924173    -0.078729    -0.954171      21.20
 C      -2.144500     1.133857    -0.538894       2.92
 O      -2.698404     2.269259    -0.281744     106.94
 C      -4.303949     2.316012    -0.485130      83.24
 H      -4.829770     1.409416     0.039015      22.08
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 H      -4.754658     3.318475    -0.236390      23.84
 H      -4.908664     1.893822    -1.607041      20.91
 C      -0.667453     1.087823    -0.280755      -8.07
 O      -0.079653     2.299025     0.294456     126.55
 C      -0.148775    -0.167866    -0.224869      49.48
 H       0.986203    -0.219611    -0.279462      19.18
 C      -2.236897    -1.376485    -0.714429     -18.75
 C      -3.204357    -2.728029    -1.057804      67.00
 H      -3.997034    -2.044816    -1.423539      21.64
 O      -2.470950    -3.661760    -1.894525     209.27
 H      -2.879693    -4.642055    -1.733489      17.74
 C      -3.684138    -3.391064     0.287082      87.38
 H      -2.939716    -3.907155     0.851371      21.51
 O      -4.374449    -2.289568     1.107815     311.14
 H      -3.813535    -2.679198     2.004387      19.75
 C      -4.841712    -4.586776    -0.036242      73.11
 O      -4.247102    -5.720851    -0.800097     243.27
 H      -3.937686    -6.495724    -0.098573      26.20
 H      -5.701977    -4.046490    -0.711439      24.89
 H      -5.272559    -5.073097     0.919200      26.67
55
name = lig-etoh-frame_949
 C       2.333092     1.765061    -2.290169      69.50
 H       1.622032     2.288509    -2.975434      22.61
 C       3.417953     1.317913     0.076140      96.94
 H       3.825764     1.892572     0.807110      27.56
 C       4.079145     0.145047    -0.463891      -0.84
 O       4.856775    -0.849041     0.195025     224.32
 C       5.212896    -0.611272     1.597376     106.42
 H       4.298285    -0.571202     2.192326      27.19
 H       5.837717     0.299129     1.663930      25.40
 H       6.028527    -1.291808     2.065826      24.20
 C       3.710159    -0.292185    -1.766115      22.50
 O       4.460324    -1.441422    -2.220697     184.22
 H       4.558557    -2.077211    -1.356197      22.14
 C       3.018684     0.475487    -2.712238      19.70
 H       2.936785     0.326860    -3.690684      21.55
 C       2.632610     2.136599    -0.986482      48.04
 C       1.969582     3.413986    -0.278767     116.58
 H       2.568278     4.282327    -0.645305      18.89
 O       2.315402     3.535748     1.213397     255.41
 H       3.168717     4.124183     0.973886      26.84
 C       0.392240     3.489766    -0.588117      55.73
 H       0.038437     3.662928    -1.576214      18.34
 C      -0.308837     4.858716    -0.030272      93.77
 O       0.422669     5.967860    -0.608362     266.99
 H       0.401197     5.895239    -1.603238      30.51
 H      -0.210909     4.892503     1.102237      23.55
 H      -1.378047     4.982170    -0.266498      24.16
 C      -0.924732    -1.478108    -0.365185      -1.65
 H      -0.227275    -2.400725    -0.266971      20.94
 C      -2.816381    -0.101188    -0.791807      73.98
 H      -3.931121    -0.067931    -0.744557      24.80
 C      -2.077653     1.043882    -0.484638      -4.63
 O      -2.752110     2.314704    -0.266473     104.60
 C      -4.308604     2.274906    -0.535167     104.74
 H      -4.616629     1.627782     0.282947      26.46
 H      -4.407130     3.241946     0.045384      23.92
 H      -4.851444     1.856866    -1.513542      24.13
 C      -0.678702     1.149734    -0.352511      10.28
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 O      -0.149103     2.234200     0.321565     109.76
 C      -0.103639    -0.137019    -0.200268      -0.73
 H       0.910771    -0.422901    -0.211108      20.23
 C      -2.307027    -1.335611    -0.660904       1.11
 C      -3.166095    -2.696320    -1.031263      77.93
 H      -4.024519    -2.104054    -1.384762      21.76
 O      -2.402824    -3.656677    -1.943728     215.44
 H      -2.688859    -4.567553    -1.671429      18.92
 C      -3.771523    -3.327382     0.254323      90.13
 H      -3.039240    -4.106218     0.725731      19.42
 O      -4.297951    -2.348487     1.055226     339.03
 H      -4.195493    -2.601631     2.034145      23.18
 C      -4.779782    -4.556921    -0.043284      99.73
 O      -4.275681    -5.749328    -0.818502     348.62
 H      -3.780731    -6.248965    -0.268789      35.57
 H      -5.737122    -4.300015    -0.469312      27.92
 H      -5.191765    -4.873215     0.923023      29.27
55
name = lig-etoh-frame_950
 C       2.347662     1.674605    -2.247337      60.34
 H       1.583341     2.244760    -2.740447      25.74
 C       3.494442     1.355423     0.011207      77.58
 H       3.710554     1.900872     1.054452      21.98
 C       3.993040     0.103080    -0.501655       5.92
 O       4.845528    -0.791542     0.175681     195.07
 C       5.204277    -0.559489     1.668532     100.47
 H       4.189225    -0.798642     2.267577      24.31
 H       5.712336     0.386541     1.919905      25.49
 H       5.815184    -1.415186     1.866519      25.29
 C       3.776038    -0.324369    -1.841828      31.32
 O       4.454771    -1.407308    -2.168504     210.00
 H       4.492232    -2.132208    -1.385512      22.83
 C       3.009790     0.508090    -2.673411      48.04
 H       2.883421    -0.017286    -3.778544      17.96
 C       2.682804     2.147543    -0.955693      94.21
 C       1.998363     3.404021    -0.352273     115.34
 H       2.562533     4.388314    -0.543999      15.56
 O       2.371167     3.574422     1.184787     271.35
 H       2.885331     4.379052     1.215955      29.90
 C       0.399051     3.502012    -0.528778      46.07
 H      -0.028976     3.380817    -1.601424      17.24
 C      -0.275334     4.855578     0.015871      89.29
 O       0.475620     5.978939    -0.664298     249.38
 H       0.543886     5.906012    -1.679805      28.18
 H      -0.217811     5.039476     1.082112      23.67
 H      -1.362120     4.793941    -0.320904      22.85
 C      -0.974369    -1.408023    -0.382681      51.48
 H      -0.377581    -2.244849    -0.430116      23.29
 C      -2.844908    -0.041558    -0.837337      44.09
 H      -3.884461     0.039737    -0.693149      24.66
 C      -2.059163     1.020588    -0.442054     -12.24
 O      -2.831001     2.333298    -0.289817      99.66
 C      -4.242227     2.250970    -0.463528      88.70
 H      -4.532466     1.698332     0.487445      24.22
 H      -4.406620     3.303166    -0.147465      23.86
 H      -4.764447     1.918504    -1.819763      21.14
 C      -0.697582     1.153793    -0.373702       2.87
 O      -0.201286     2.215880     0.307037     114.58
 C      -0.092316    -0.211522    -0.212891       9.59
 H       1.028889    -0.392302     0.028911      19.44
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 C      -2.307918    -1.428625    -0.625605      11.82
 C      -3.117173    -2.619805    -0.984374      76.62
 H      -4.015773    -2.527059    -1.749149      18.92
 O      -2.355471    -3.618417    -1.968980     215.85
 H      -2.605883    -4.465135    -1.638344      22.36
 C      -3.821574    -3.374769     0.189260      86.15
 H      -2.948073    -3.829872     0.672131      20.75
 O      -4.248375    -2.386764     1.006751     335.14
 H      -4.345551    -2.475070     2.057059      22.22
 C      -4.746928    -4.536783    -0.047601      84.32
 O      -4.308780    -5.740380    -0.834615     294.80
 H      -3.436681    -6.138388    -0.253342      25.74
 H      -5.787893    -4.365978    -0.554488      24.42
 H      -4.969380    -4.775119     1.055478      26.71
55
name = lig-etoh-frame_951
 C       2.384416     1.593125    -2.169222      33.40
 H       1.609105     2.136181    -2.758233      21.31
 C       3.566031     1.404096    -0.092998      89.49
 H       3.534080     1.551616     0.955537      18.40
 C       3.916526     0.103781    -0.488676      55.41
 O       4.842483    -0.719409     0.190161     227.58
 C       5.156365    -0.541304     1.710402     104.59
 H       4.308042    -0.745776     2.276840      31.93
 H       5.458393     0.478871     2.033847      28.97
 H       5.711357    -1.534554     1.669354      25.74
 C       3.823185    -0.289945    -1.859730      23.89
 O       4.461211    -1.432277    -2.164489     247.92
 H       4.489618    -1.931860    -1.443764      29.18
 C       2.991493     0.488922    -2.699370      44.62
 H       2.777896    -0.021293    -3.554804      24.38
 C       2.724870     2.146531    -0.863860      72.91
 C       2.036895     3.426685    -0.383552     101.25
 H       2.322115     4.341121    -0.924375      17.23
 O       2.399245     3.597562     1.133073     314.22
 H       2.655134     4.498442     1.450258      30.44
 C       0.406319     3.498650    -0.447081      56.13
 H       0.171402     3.049333    -1.399898      17.13
 C      -0.220078     4.840134     0.007679      95.58
 O       0.514850     5.991531    -0.692093     220.87
 H       0.524638     5.680192    -1.753588      24.05
 H      -0.125749     5.131305     1.076530      22.12
 H      -1.234804     4.705278    -0.308211      22.88
 C      -0.925664    -1.315520    -0.392252      53.07
 H      -0.497325    -2.425598    -0.497680      20.94
 C      -2.872986    -0.061258    -0.833863      25.59
 H      -4.008202     0.157433    -0.821238      22.73
 C      -2.142956     1.087486    -0.442222     -13.81
 O      -2.856998     2.315668    -0.333993     206.25
 C      -4.191518     2.257641    -0.377868     140.18
 H      -4.772691     1.604735     0.286379      26.62
 H      -4.699414     3.308885    -0.609136      24.32
 H      -4.361475     2.089110    -1.296600      28.84
 C      -0.675204     1.058056    -0.332097     -10.21
 O      -0.217234     2.254004     0.282008     113.98
 C      -0.114705    -0.272845    -0.244282      64.22
 H       0.851540    -0.248809     0.139060      19.55
 C      -2.333567    -1.442593    -0.641142       4.60
 C      -3.127313    -2.604964    -1.020950      92.77
 H      -3.742710    -2.519151    -1.842495      19.24
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 O      -2.305203    -3.555268    -1.964790     170.83
 H      -2.573277    -4.527875    -1.614820      20.56
 C      -3.757420    -3.447842     0.120207      85.40
 H      -2.793639    -3.720801     0.676008      19.71
 O      -4.256821    -2.366380     0.961030     303.11
 H      -4.131905    -2.654233     2.056759      21.23
 C      -4.770753    -4.556411    -0.048575      90.37
 O      -4.306817    -5.717383    -0.815132     335.81
 H      -3.404934    -5.979798    -0.477696      29.28
 H      -5.695891    -4.233743    -0.598870      24.78
 H      -4.818545    -4.847941     1.014599      27.32
55
name = lig-etoh-frame_952
 C       2.401704     1.580765    -2.082477      26.79
 H       1.722423     1.994696    -2.811607      21.64
 C       3.621686     1.409042    -0.139938      94.05
 H       3.590824     1.462923     0.979382      18.97
 C       3.901437     0.118818    -0.486813      72.56
 O       4.832412    -0.635874     0.235978     252.32
 C       5.088405    -0.556050     1.691300     104.63
 H       4.095342    -0.733803     2.390246      27.40
 H       5.462630     0.439485     1.956840      28.76
 H       5.879303    -1.303106     1.819817      27.45
 C       3.847532    -0.224827    -1.822039      18.74
 O       4.471917    -1.480730    -2.217289     157.34
 H       4.646147    -1.888230    -1.175947      20.22
 C       2.995035     0.423750    -2.708214      34.00
 H       2.576502     0.069011    -3.761810      21.94
 C       2.714473     2.159479    -0.831971      87.49
 C       2.060127     3.481534    -0.344387      90.98
 H       2.158146     4.162925    -1.303970      19.30
 O       2.410276     3.603448     1.054584     327.68
 H       2.407897     4.580413     1.422332      28.86
 C       0.461977     3.417809    -0.374711      78.41
 H       0.291939     3.198055    -1.474044      17.29
 C      -0.139265     4.832825    -0.032449      96.09
 O       0.530140     5.968769    -0.721960     280.47
 H       0.475146     5.727411    -1.618901      31.93
 H      -0.018946     5.039477     1.054892      23.42
 H      -1.275641     4.831968    -0.266501      22.67
 C      -0.909300    -1.387884    -0.426464      54.65
 H      -0.496329    -2.317141    -0.362266      23.90
 C      -2.927242    -0.110075    -0.784932      56.11
 H      -3.916942    -0.010640    -1.084806      26.50
 C      -2.222069     1.139020    -0.483703      -1.69
 O      -2.799143     2.303339    -0.349559     141.28
 C      -4.226099     2.320490    -0.293094      91.01
 H      -4.932113     1.575407     0.139560      24.27
 H      -4.701013     3.182281    -0.519435      26.17
 H      -4.447794     1.699510    -1.788357      20.16
 C      -0.721506     0.991175    -0.254574     -28.75
 O      -0.207221     2.298695     0.282577     148.25
 C      -0.124239    -0.222406    -0.260807      55.84
 H       0.942658    -0.295568     0.138871      18.39
 C      -2.333425    -1.320125    -0.685509      -4.49
 C      -3.141413    -2.668135    -1.121760      78.06
 H      -3.925622    -2.036913    -1.850983      18.83
 O      -2.244518    -3.506229    -1.933685     221.43
 H      -2.466636    -4.427659    -1.770085      22.84
 C      -3.630936    -3.451846     0.081380      95.72
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 H      -2.790393    -3.943061     0.611753      22.01
 O      -4.283128    -2.355912     0.937174     315.55
 H      -3.967972    -2.614764     1.823394      26.18
 C      -4.768231    -4.592415    -0.047983      91.91
 O      -4.295574    -5.688688    -0.806797     356.68
 H      -3.439695    -5.961833    -0.522225      31.30
 H      -5.677784    -4.114363    -0.492025      25.32
 H      -5.045020    -4.978599     0.977456      26.67
55
name = lig-etoh-frame_953
 C       2.403905     1.583762    -2.066243      28.34
 H       1.702585     2.084093    -2.767910      20.44
 C       3.634536     1.409376    -0.074553      67.72
 H       3.908269     1.746246     0.984223      17.04
 C       3.964422     0.143397    -0.483100      48.97
 O       4.825482    -0.581883     0.293620     281.93
 C       4.999350    -0.554994     1.670151     129.30
 H       4.173343    -0.758295     2.208130      32.33
 H       5.487919     0.431582     1.867215      28.17
 H       5.927304    -1.101560     2.047552      27.46
 C       3.874108    -0.261900    -1.842829      29.54
 O       4.468928    -1.519160    -2.233294     204.37
 H       4.990295    -1.760582    -1.419365      22.91
 C       2.979761     0.387707    -2.681708      50.08
 H       2.650414     0.309465    -3.729952      25.51
 C       2.674339     2.184564    -0.849254      51.04
 C       2.040230     3.487073    -0.315903     116.50
 H       2.316986     4.177767    -1.075670      20.84
 O       2.423253     3.628913     0.975676     375.81
 H       2.251844     4.517024     1.205139      32.62
 C       0.530561     3.318205    -0.396788      92.35
 H       0.319306     3.530918    -1.464547      18.47
 C      -0.077293     4.826069    -0.061302     102.94
 O       0.535181     5.925792    -0.722783     264.05
 H       0.433158     5.867652    -1.861017      24.43
 H       0.076555     4.941842     1.019112      24.76
 H      -1.117140     4.933824    -0.199630      25.01
 C      -0.932475    -1.468449    -0.466167       5.68
 H      -0.320892    -2.453275    -0.219140      20.08
 C      -2.988402    -0.079472    -0.728700      46.19
 H      -3.983423    -0.232413    -1.305847      16.69
 C      -2.225799     1.075081    -0.529532      14.40
 O      -2.767469     2.337809    -0.335070     151.76
 C      -4.288416     2.316801    -0.366098      97.50
 H      -4.741782     1.536201     0.297282      23.99
 H      -4.616469     3.505421    -0.279383      22.90
 H      -4.609215     1.757726    -1.372095      21.94
 C      -0.851758     1.049681    -0.174085       2.91
 O      -0.192967     2.315517     0.313250     169.16
 C      -0.103449    -0.184450    -0.246740     -18.06
 H       0.937704    -0.362025    -0.081731      20.79
 C      -2.267956    -1.267644    -0.746644       4.20
 C      -3.139801    -2.678462    -1.250217      79.01
 H      -3.971125    -2.166361    -1.541037      25.16
 O      -2.184154    -3.449786    -1.907038     240.99
 H      -2.456325    -4.368791    -1.925758      23.30
 C      -3.573380    -3.428968     0.083117      83.19
 H      -2.753081    -4.026217     0.549138      22.84
 O      -4.300578    -2.378177     0.894449     247.16
 H      -3.780900    -2.376822     1.971475      21.76
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 C      -4.730430    -4.600291    -0.025631      88.11
 O      -4.290884    -5.670343    -0.833534     288.14
 H      -3.379666    -6.104873    -0.319657      25.35
 H      -5.671700    -4.060583    -0.491678      24.60
 H      -5.265532    -4.944077     0.912951      25.92
55
name = lig-etoh-frame_954
 C       2.380016     1.598534    -2.117531      27.81
 H       1.667974     2.208907    -2.661036      20.67
 C       3.595391     1.462067     0.024879      49.10
 H       4.139165     1.987234     0.797906      22.25
 C       4.070802     0.191751    -0.473816      17.27
 O       4.844091    -0.594729     0.315009     232.27
 C       4.974682    -0.491565     1.672805     110.03
 H       3.928231    -0.835485     2.247391      25.51
 H       5.204316     0.550431     1.987105      24.99
 H       5.743416    -1.214681     2.044575      25.00
 C       3.891277    -0.371161    -1.885798      21.76
 O       4.470018    -1.532809    -2.241065     219.54
 H       5.259334    -1.723302    -1.669216      25.22
 C       2.956094     0.422916    -2.613060      70.11
 H       2.858422     0.271408    -3.712653      27.29
 C       2.679714     2.165071    -0.848447      52.42
 C       2.014117     3.407403    -0.346949     122.62
 H       2.501681     4.457761    -0.733004      16.76
 O       2.448704     3.665564     0.946771     370.51
 H       2.200683     4.585573     1.141171      30.38
 C       0.546287     3.315500    -0.498787      76.47
 H       0.238492     3.323543    -1.553284      19.29
 C      -0.022173     4.792998    -0.052948      94.17
 O       0.551910     5.893470    -0.750418     298.07
 H       0.420082     5.845492    -1.650021      32.84
 H       0.209791     4.984815     1.039758      23.77
 H      -1.179679     4.801038    -0.197574      23.14
 C      -0.883559    -1.466878    -0.476286      48.08
 H      -0.422136    -2.418412    -0.298123      22.58
 C      -3.037624    -0.059931    -0.717957      36.01
 H      -3.953031    -0.152031    -1.228300      17.17
 C      -2.235224     1.043670    -0.535669       9.51
 O      -2.787674     2.379557    -0.327089     111.43
 C      -4.301838     2.347732    -0.411974      97.30
 H      -4.435161     1.769713     0.576844      23.78
 H      -4.453662     3.259820    -0.068400      27.02
 H      -5.085085     1.892091    -1.451564      20.54
 C      -0.904016     1.112628    -0.105450      -0.27
 O      -0.189270     2.299591     0.353057     138.40
 C      -0.154252    -0.189241    -0.230361      -2.34
 H       0.975160    -0.231570    -0.241012      20.95
 C      -2.228726    -1.334539    -0.828527     -12.49
 C      -3.091071    -2.641146    -1.252091      62.32
 H      -4.234784    -2.498553    -1.784445      22.41
 O      -2.121184    -3.405268    -1.912498     196.44
 H      -2.579511    -4.353933    -2.143093      20.17
 C      -3.594850    -3.410767     0.113740      85.20
 H      -2.624629    -3.804664     0.569752      23.07
 O      -4.273764    -2.414873     0.884337     392.56
 H      -4.019162    -2.238877     1.672138      34.57
 C      -4.701615    -4.550309    -0.016239      96.22
 O      -4.252767    -5.679133    -0.861082     357.37
 H      -3.736841    -6.176047    -0.294194      32.38
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 H      -5.496940    -4.153683    -0.626121      26.51
 H      -5.108856    -4.837704     0.953268      26.61
55
name = lig-etoh-frame_955
 C       2.348227     1.640990    -2.143573      42.68
 H       1.653541     2.213932    -2.774424      22.14
 C       3.553834     1.495769     0.065058     102.02
 H       4.251933     2.181131     0.707122      28.60
 C       4.168184     0.250882    -0.487541       4.02
 O       4.891006    -0.647691     0.294680     196.16
 C       4.916021    -0.420320     1.751596     108.93
 H       4.014937    -0.738999     2.091422      30.41
 H       4.954807     0.586546     2.174928      25.17
 H       5.585203    -1.263150     1.968839      24.12
 C       3.871025    -0.396874    -1.829913      12.73
 O       4.472391    -1.562850    -2.260784     149.56
 H       5.557663    -1.614712    -1.948926      24.72
 C       2.959608     0.447177    -2.577592      43.93
 H       3.029524     0.076299    -3.684906      22.65
 C       2.717731     2.106304    -0.842868      44.25
 C       2.044860     3.356139    -0.414917     124.67
 H       2.290597     4.246221    -0.857219      19.59
 O       2.467580     3.687404     0.985321     342.08
 H       2.251217     4.691529     1.181742      29.73
 C       0.486941     3.381023    -0.618447      34.68
 H       0.164574     2.884541    -1.592490      17.95
 C      -0.006025     4.735236    -0.034100     101.21
 O       0.578777     5.874581    -0.750685     258.45
 H       0.381619     5.675289    -1.851212      23.45
 H       0.266893     4.955068     0.976637      22.91
 H      -1.045718     4.600277    -0.130188      23.55
 C      -0.831835    -1.385638    -0.479706      53.29
 H      -0.399959    -2.438331    -0.491611      20.34
 C      -3.001751    -0.125821    -0.750351      26.40
 H      -4.089748     0.080287    -1.065457      16.71
 C      -2.273195     1.119065    -0.482783     -11.95
 O      -2.840461     2.395618    -0.366729     136.29
 C      -4.282686     2.363900    -0.385388      94.47
 H      -4.455918     1.890344     0.601773      23.28
 H      -4.589289     3.535446    -0.018885      22.20
 H      -5.150791     2.071183    -1.453809      19.28
 C      -0.846914     1.101000    -0.065475      -1.28
 O      -0.192504     2.268053     0.386266     116.83
 C      -0.237429    -0.180767    -0.209383      50.16
 H       0.842897    -0.013696    -0.224804      21.28
 C      -2.283069    -1.400548    -0.906667      11.83
 C      -3.077290    -2.596044    -1.189728      88.75
 H      -3.749354    -2.698367    -1.983031      23.91
 O      -2.070671    -3.406886    -1.946132     250.79
 H      -2.560225    -4.135589    -2.264439      26.49
 C      -3.609994    -3.386082     0.150282      87.12
 H      -2.672855    -3.586529     0.650326      23.47
 O      -4.269913    -2.439331     0.845616     333.27
 H      -4.012195    -2.231516     1.952305      22.77
 C      -4.641145    -4.490582    -0.045550      78.53
 O      -4.218015    -5.684062    -0.880179     301.09
 H      -3.835663    -6.416705    -0.238047      26.99
 H      -5.523415    -4.129122    -0.789721      23.72
 H      -4.859923    -4.753989     1.048759      24.86
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name = lig-etoh-frame_956
 C       2.342283     1.654769    -2.150040      50.70
 H       1.733794     2.147200    -2.914357      23.23
 C       3.596356     1.470889     0.047084     122.32
 H       4.013436     2.108268     0.740975      30.63
 C       4.238767     0.268708    -0.500804      23.75
 O       4.949988    -0.674242     0.272293     170.84
 C       4.848332    -0.378840     1.817927      71.83
 H       3.719096    -0.770724     2.055788      23.93
 H       5.063012     0.639124     2.235222      23.64
 H       5.653989    -1.131455     2.191035      24.45
 C       3.830941    -0.311929    -1.699502      21.45
 O       4.493023    -1.590600    -2.287345     210.76
 H       5.363828    -1.473212    -2.175139      31.88
 C       3.010452     0.420566    -2.591615      24.26
 H       2.892240     0.072496    -3.565355      21.39
 C       2.716991     2.074512    -0.862618      44.92
 C       2.063400     3.342513    -0.449753      86.09
 H       2.266465     4.133156    -1.415218      17.19
 O       2.462869     3.696641     1.027005     353.82
 H       2.422090     4.631613     1.143033      31.40
 C       0.439157     3.396002    -0.682889      43.02
 H       0.106165     2.877619    -1.550020      18.42
 C      -0.007101     4.674353    -0.056886      87.37
 O       0.585437     5.846602    -0.771495     266.69
 H       0.523586     5.614938    -1.737490      28.15
 H       0.333592     4.717956     1.041205      20.67
 H      -1.176925     4.642303    -0.031745      21.51
 C      -0.877171    -1.338228    -0.515219      41.35
 H      -0.193881    -2.233597    -0.752738      19.42
 C      -2.932164    -0.163033    -0.811708      50.38
 H      -3.997569     0.074198    -0.776011      23.37
 C      -2.271799     1.179094    -0.393002     -23.16
 O      -2.904888     2.397731    -0.441836     184.61
 C      -4.293429     2.458933    -0.286378     128.40
 H      -4.807119     1.742152     0.446349      23.94
 H      -4.613807     3.417430    -0.322646      27.16
 H      -4.775114     2.177478    -1.291710      23.51
 C      -0.843365     1.088558    -0.064292       7.74
 O      -0.190832     2.234274     0.412617      88.83
 C      -0.270208    -0.127890    -0.176340      61.54
 H       0.809948    -0.053759    -0.032757      21.51
 C      -2.329834    -1.367765    -0.925521      14.47
 C      -3.040842    -2.629405    -1.135100      87.48
 H      -3.709873    -2.400088    -2.118339      19.27
 O      -2.014091    -3.433946    -1.967358     220.11
 H      -2.542117    -4.154551    -2.378784      23.79
 C      -3.571572    -3.345545     0.137298      94.84
 H      -2.655094    -3.702781     0.774124      21.77
 O      -4.306701    -2.392234     0.868230     314.82
 H      -4.051000    -2.677356     1.830108      24.14
 C      -4.570048    -4.475490    -0.111184     102.30
 O      -4.180036    -5.679356    -0.879075     301.63
 H      -3.861185    -6.525372    -0.286410      26.67
 H      -5.430499    -4.056841    -0.516657      28.44
 H      -4.845058    -4.732872     0.885254      28.10
55
name = lig-etoh-frame_957
 C       2.392069     1.585943    -2.177549      67.57
 H       1.809905     2.157858    -2.905018      24.24
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 C       3.672922     1.407570    -0.039694      57.44
 H       3.752212     1.936954     1.041367      19.77
 C       4.289920     0.250771    -0.448304      27.06
 O       5.018770    -0.658023     0.290891     211.57
 C       4.778104    -0.387311     1.855716     102.55
 H       3.809334    -0.611084     2.075879      30.18
 H       5.129111     0.609879     2.051435      25.83
 H       5.510525    -0.911792     2.416157      27.29
 C       3.815506    -0.246674    -1.648318      36.10
 O       4.465388    -1.573295    -2.295950     134.08
 H       5.493011    -1.346417    -2.243823      25.76
 C       3.049678     0.420528    -2.584817      35.87
 H       2.647085     0.010843    -3.639964      21.59
 C       2.684820     2.074236    -0.879082      38.83
 C       2.050060     3.384422    -0.492942     110.06
 H       2.423728     3.891037    -1.275392      20.12
 O       2.437773     3.688171     1.010204     308.29
 H       2.636458     4.652968     1.055541      28.60
 C       0.441726     3.333649    -0.654358      49.22
 H       0.022782     3.152592    -1.716387      18.51
 C      -0.054167     4.640803    -0.085685     100.32
 O       0.579480     5.806300    -0.760206     252.55
 H       0.595805     5.643132    -1.850155      25.79
 H       0.350974     4.489465     0.885027      22.00
 H      -1.084397     4.858526     0.008343      24.48
 C      -0.950490    -1.302054    -0.587969      69.27
 H      -0.203306    -2.011763    -0.797002      28.40
 C      -2.885861    -0.060531    -0.834987      23.86
 H      -3.980204    -0.202863    -0.723285      26.56
 C      -2.248268     1.149715    -0.327447       1.71
 O      -2.949516     2.398314    -0.501312     150.68
 C      -4.311166     2.537031    -0.172135      76.40
 H      -5.010627     1.776977     0.226568      22.40
 H      -4.626603     3.667375    -0.295941      22.38
 H      -4.818717     1.963696    -1.725523      20.83
 C      -0.925130     1.159057    -0.073350      12.15
 O      -0.175981     2.214714     0.425309     114.52
 C      -0.245364    -0.113524    -0.144156      18.86
 H       0.814393    -0.283934     0.205139      23.89
 C      -2.280321    -1.313863    -0.882864     -21.83
 C      -2.994107    -2.682153    -1.177475     107.86
 H      -3.870293    -2.225950    -1.631482      20.70
 O      -1.977110    -3.478834    -1.956462     216.11
 H      -2.513138    -4.266501    -2.444947      19.37
 C      -3.499798    -3.318937     0.096738     105.97
 H      -2.736322    -3.785952     0.657551      24.05
 O      -4.349200    -2.341182     0.913972     264.92
 H      -4.264510    -2.743979     1.864105      23.96
 C      -4.485122    -4.509837    -0.162380      86.54
 O      -4.145493    -5.667260    -0.884264     337.10
 H      -3.801277    -6.257060    -0.323445      33.05
 H      -5.533975    -3.915547    -0.445560      25.51
 H      -4.926403    -4.871944     0.863911      26.82
55
name = lig-etoh-frame_958
 C       2.456044     1.535120    -2.191561      54.24
 H       1.818314     2.144624    -2.835632      21.88
 C       3.699857     1.417700    -0.090550      96.82
 H       3.584236     1.513543     0.919173      20.41
 C       4.319190     0.193158    -0.385886      24.73
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 O       5.093437    -0.629188     0.369999     231.54
 C       4.765298    -0.384445     1.834029      96.78
 H       3.623536    -0.499894     2.157625      27.03
 H       4.998664     0.729102     1.850491      24.08
 H       5.397757    -1.049269     2.606448      24.36
 C       3.862860    -0.277520    -1.707276      26.73
 O       4.421327    -1.504841    -2.273221     149.70
 H       5.506219    -1.355351    -2.270844      26.00
 C       3.045067     0.416409    -2.600929      32.04
 H       2.758465     0.022147    -3.452315      25.21
 C       2.679501     2.048146    -0.886780      80.45
 C       2.014879     3.380622    -0.478136     122.84
 H       2.650303     4.265398    -1.119396      19.18
 O       2.390489     3.679635     0.934089     273.28
 H       2.957313     4.570564     0.943233      28.66
 C       0.437211     3.253237    -0.608859      78.53
 H       0.124984     3.303770    -1.631955      19.56
 C      -0.090697     4.634408    -0.112677      92.40
 O       0.573636     5.757348    -0.740142     267.02
 H       0.546175     5.703878    -1.788238      28.61
 H       0.360574     4.600825     0.948752      21.77
 H      -1.201961     4.897070    -0.060468      23.67
 C      -0.921968    -1.219896    -0.637123      76.22
 H      -0.280082    -2.266435    -0.707541      25.50
 C      -2.897249     0.048482    -0.814930      44.46
 H      -3.967953    -0.248340    -0.873410      23.78
 C      -2.313102     1.122746    -0.323053      20.47
 O      -2.973234     2.395535    -0.512751     215.06
 C      -4.366950     2.587104    -0.222758     121.64
 H      -4.944238     1.866818     0.327481      25.86
 H      -4.563374     3.669391    -0.056456      26.04
 H      -4.820979     2.162842    -1.274195      23.46
 C      -0.920029     1.203877    -0.060740       0.30
 O      -0.148313     2.234264     0.405500     150.75
 C      -0.245483    -0.121721    -0.117760      34.26
 H       0.712602    -0.323057     0.275296      24.66
 C      -2.229731    -1.280108    -0.843546     -34.44
 C      -2.929376    -2.664942    -1.227392      99.89
 H      -4.065501    -2.422638    -1.457089      21.35
 O      -1.991324    -3.532744    -1.929840     267.02
 H      -2.418014    -4.250406    -2.317576      24.87
 C      -3.462184    -3.326551     0.083015      69.72
 H      -2.541546    -3.746499     0.703407      21.94
 O      -4.355571    -2.313017     0.934608     202.16
 H      -4.596062    -2.595193     2.030556      22.80
 C      -4.480025    -4.518812    -0.156579     107.89
 O      -4.111500    -5.641743    -0.925403     320.37
 H      -3.483585    -6.182647    -0.195529      25.28
 H      -5.274097    -4.129298    -0.642648      28.67
 H      -4.750268    -4.890212     0.786816      27.75
55
name = lig-etoh-frame_959
 C       2.477773     1.579763    -2.172816      23.96
 H       1.763096     2.057706    -2.846771      20.55
 C       3.681107     1.422602    -0.104256      84.66
 H       3.542172     1.517635     1.040451      18.79
 C       4.296506     0.124774    -0.426123      15.58
 O       5.157052    -0.611367     0.482340     259.44
 C       4.764638    -0.359693     1.818058     128.07
 H       3.710229    -0.477037     1.970121      30.54
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 H       4.916312     0.669364     2.033331      26.97
 H       5.241578    -1.043636     2.381961      28.92
 C       3.975800    -0.347313    -1.768629      26.46
 O       4.392194    -1.432847    -2.245268     241.88
 H       5.255127    -1.491371    -2.213281      32.62
 C       3.065218     0.372805    -2.595559      40.76
 H       2.924747    -0.021042    -3.693197      27.18
 C       2.710308     2.023330    -0.905370      79.03
 C       2.028328     3.364696    -0.450596     141.06
 H       2.243259     4.266480    -0.849008      23.10
 O       2.342481     3.678419     0.848370     321.28
 H       3.130341     4.195890     0.865821      32.79
 C       0.428486     3.238925    -0.547809      73.96
 H       0.170618     2.974968    -1.638795      20.74
 C      -0.115732     4.646389    -0.090917     104.16
 O       0.569974     5.721654    -0.716891     310.74
 H       0.446420     5.637575    -1.720006      28.49
 H       0.112864     4.896760     0.927853      24.47
 H      -1.208590     4.613092    -0.225148      24.84
 C      -0.798353    -1.211509    -0.652553      57.35
 H      -0.500449    -2.168862    -0.575541      27.75
 C      -2.966057    -0.011635    -0.798134      63.11
 H      -4.026058     0.138575    -1.079240      25.43
 C      -2.376840     1.212689    -0.340432      -2.01
 O      -2.977353     2.400269    -0.488295     155.62
 C      -4.402416     2.603157    -0.285843      97.67
 H      -4.637255     2.031992     0.754649      23.65
 H      -4.531531     3.643382     0.131281      25.04
 H      -5.357184     2.547298    -1.285760      21.57
 C      -0.858733     1.157358    -0.041521      -4.92
 O      -0.113795     2.285550     0.360486     175.10
 C      -0.270465    -0.074678    -0.093414      56.46
 H       0.808583    -0.159618     0.268389      22.63
 C      -2.252871    -1.230443    -0.853947     -14.65
 C      -2.915971    -2.595734    -1.215213      88.09
 H      -3.779765    -2.636423    -1.912607      22.38
 O      -2.022831    -3.566005    -1.890387     226.76
 H      -2.546101    -4.381873    -2.171697      20.60
 C      -3.428673    -3.360694     0.144110      82.48
 H      -2.580144    -3.534293     0.715165      24.18
 O      -4.345021    -2.301567     0.933940     295.68
 H      -4.444059    -2.518609     1.760177      31.33
 C      -4.468705    -4.501372    -0.133933      76.02
 O      -4.038853    -5.647158    -0.955296     327.64
 H      -3.187431    -6.073040    -0.558076      26.82
 H      -5.340182    -4.179597    -0.934449      22.44
 H      -4.720312    -4.839104     0.962465      24.56
55
name = lig-etoh-frame_960
 C       2.481914     1.597894    -2.200535      36.83
 H       1.730996     2.029895    -2.868539      21.97
 C       3.655886     1.352224    -0.060071      24.41
 H       3.697248     1.866540     0.917340      18.75
 C       4.255857     0.100609    -0.487435       7.24
 O       5.194772    -0.585157     0.539121     210.36
 C       4.753425    -0.314977     1.813000      94.92
 H       3.614395    -0.589997     1.793991      26.11
 H       5.033740     0.629686     2.420278      23.88
 H       5.347056    -1.211629     2.414335      24.69
 C       4.046472    -0.295535    -1.763144      39.21
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 O       4.394279    -1.476800    -2.267816     182.26
 H       5.424576    -1.796080    -2.046966      23.69
 C       3.095781     0.340579    -2.599431      64.02
 H       3.165423     0.188204    -3.666372      30.82
 C       2.751557     2.062931    -0.911901      41.96
 C       2.010360     3.299042    -0.438971     114.87
 H       1.975723     4.308704    -1.244730      16.24
 O       2.307161     3.675214     0.829620     307.64
 H       3.295307     3.872595     0.874656      29.28
 C       0.446331     3.263763    -0.512206      68.71
 H       0.195209     2.754740    -1.430040      20.73
 C      -0.149497     4.646603    -0.066287      94.40
 O       0.561445     5.707288    -0.704919     268.66
 H       0.360846     5.579564    -1.801236      23.39
 H      -0.194508     4.921505     1.041775      22.86
 H      -1.214129     4.448207    -0.422684      22.47
 C      -0.781699    -1.222343    -0.647652      34.00
 H      -0.298579    -2.356368    -0.419393      23.70
 C      -3.057334    -0.062927    -0.773675      46.05
 H      -3.967594     0.335871    -1.260189      21.87
 C      -2.350454     1.257443    -0.375373     -15.46
 O      -2.992847     2.445258    -0.470343     107.57
 C      -4.446790     2.620854    -0.265275      92.80
 H      -4.483202     2.163981     0.663037      24.93
 H      -4.410917     3.728498     0.109321      23.58
 H      -5.518819     2.628638    -1.250241      19.70
 C      -0.879221     1.157658    -0.035312       4.30
 O      -0.095991     2.311888     0.343401     145.95
 C      -0.217431    -0.036344    -0.063944      44.76
 H       0.810544     0.097273     0.146690      22.60
 C      -2.254543    -1.197439    -0.902089      -3.42
 C      -2.944633    -2.557301    -1.181557      85.49
 H      -3.451580    -2.475428    -2.210929      19.92
 O      -2.036971    -3.594569    -1.847386     174.74
 H      -2.760525    -4.386032    -1.844604      16.54
 C      -3.459578    -3.325151     0.190193      73.65
 H      -2.504593    -3.509002     0.881814      21.28
 O      -4.305746    -2.304183     0.871631     232.08
 H      -4.150691    -2.645398     2.004590      21.86
 C      -4.447563    -4.495773    -0.120192      98.74
 O      -3.936057    -5.654819    -0.985220     375.60
 H      -3.089402    -6.022514    -0.773541      29.74
 H      -5.246074    -4.116374    -0.620174      27.85
 H      -4.888467    -4.764555     0.797489      28.03
55
name = lig-etoh-frame_961
 C       2.498374     1.553383    -2.248857      41.37
 H       1.792291     2.089706    -2.896104      20.57
 C       3.613987     1.294261    -0.029756      43.01
 H       3.999100     1.906900     0.807079      22.63
 C       4.255585     0.138248    -0.433568      21.89
 O       5.211861    -0.530363     0.501489     215.04
 C       4.740426    -0.334030     1.888733     116.55
 H       3.678730    -0.573097     1.875972      28.62
 H       5.034815     0.503291     2.453117      26.72
 H       5.186024    -1.088590     2.376253      29.22
 C       4.073118    -0.236079    -1.776958      34.16
 O       4.457619    -1.594160    -2.322226     141.25
 H       5.230446    -1.992953    -1.729358      23.65
 C       3.131574     0.395745    -2.603514      60.54
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 H       3.261932     0.182515    -3.684650      28.15
 C       2.788023     2.103281    -0.918675      47.89
 C       1.956592     3.276082    -0.502460     140.29
 H       2.144530     3.805688    -1.352421      25.99
 O       2.303152     3.692187     0.861660     310.69
 H       3.329417     3.601670     0.978202      26.67
 C       0.486282     3.270227    -0.484588      71.66
 H       0.161675     3.016615    -1.550954      20.40
 C      -0.207133     4.629689    -0.069019     102.24
 O       0.532677     5.708562    -0.717205     322.49
 H       0.452747     5.664802    -1.627924      31.52
 H      -0.359260     4.673262     0.998660      25.68
 H      -1.187474     4.589451    -0.565116      23.71
 C      -0.821871    -1.246818    -0.583465      46.61
 H      -0.231305    -2.031557    -0.508654      27.51
 C      -3.081846     0.003141    -0.745782      24.59
 H      -4.021878     0.045322    -1.348559      17.18
 C      -2.299026     1.203526    -0.423996       3.65
 O      -3.005190     2.512033    -0.474896     146.31
 C      -4.458423     2.691408    -0.209409     107.00
 H      -4.822968     1.939500     0.660127      23.46
 H      -4.456827     3.758183    -0.114631      25.55
 H      -5.211435     2.351222    -0.984722      24.37
 C      -0.959750     1.236485    -0.042535       2.62
 O      -0.117355     2.285036     0.396294     137.90
 C      -0.154437    -0.042154    -0.073777      -2.81
 H       0.949188     0.178177     0.070058      22.02
 C      -2.217312    -1.213849    -0.943991     -12.09
 C      -2.948315    -2.549189    -1.177169      83.38
 H      -3.655797    -2.139310    -1.933997      23.95
 O      -2.054309    -3.630455    -1.782417     232.13
 H      -2.652999    -4.309885    -1.669142      19.50
 C      -3.504586    -3.231868     0.198551      98.46
 H      -2.681454    -3.574081     0.734265      24.72
 O      -4.251061    -2.340470     0.856860     349.36
 H      -4.001237    -2.383239     1.778750      29.54
 C      -4.379560    -4.515715    -0.106435      78.00
 O      -3.856908    -5.629130    -1.016781     318.29
 H      -2.878689    -6.062697    -0.581776      21.39
 H      -5.337414    -3.932099    -0.601626      23.39
 H      -4.988621    -4.958045     0.798521      25.02
55
name = lig-etoh-frame_962
 C       2.515198     1.549102    -2.243588      43.60
 H       1.931675     2.118330    -2.968895      22.45
 C       3.557857     1.318225    -0.015563      99.93
 H       4.253610     1.691326     0.828700      24.45
 C       4.302683     0.165030    -0.357768      30.50
 O       5.197785    -0.450795     0.431638     203.61
 C       4.728689    -0.387056     1.953097      76.34
 H       3.611134    -0.474009     2.072075      26.82
 H       4.995065     0.649447     2.326465      22.63
 H       5.227910    -1.335956     2.524577      23.64
 C       4.098114    -0.281978    -1.799388       7.91
 O       4.528525    -1.677312    -2.346728     169.46
 H       4.968649    -2.008376    -1.605437      26.55
 C       3.210602     0.454756    -2.649164      38.03
 H       3.140199    -0.018331    -3.695279      21.52
 C       2.793706     2.052872    -0.942386      57.39
 C       1.951952     3.254933    -0.524193     138.80
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 H       2.455433     3.959014    -1.441449      16.76
 O       2.316281     3.715969     0.887289     350.63
 H       3.205357     3.540714     1.060366      28.73
 C       0.452417     3.260948    -0.498526      76.29
 H       0.129246     3.354785    -1.531203      19.02
 C      -0.254322     4.603568    -0.135690      93.16
 O       0.500298     5.728594    -0.678868     263.61
 H       0.498644     5.685217    -1.833794      23.42
 H      -0.324816     4.602322     0.987924      24.26
 H      -1.260792     4.694528    -0.589651      23.55
 C      -0.861899    -1.190185    -0.479585      18.23
 H      -0.103781    -2.161122    -0.712540      18.24
 C      -3.007538     0.046972    -0.759339      29.91
 H      -3.992982    -0.199617    -1.138066      17.66
 C      -2.336628     1.184462    -0.474425      17.88
 O      -3.007698     2.558969    -0.481184     129.47
 C      -4.397333     2.711862    -0.087888      70.60
 H      -4.995571     2.158759     0.527069      24.27
 H      -4.742255     3.872372    -0.231350      22.55
 H      -5.306741     2.028037    -1.404115      19.66
 C      -0.955739     1.249598    -0.050934       3.24
 O      -0.165470     2.247437     0.472906     127.97
 C      -0.167550    -0.016789    -0.126168      12.89
 H       0.907077    -0.007983     0.032553      23.30
 C      -2.187467    -1.226695    -0.936158      -5.53
 C      -2.931327    -2.547230    -1.182236      70.30
 H      -4.023782    -2.220699    -1.540672      24.28
 O      -2.080000    -3.623641    -1.711806     169.51
 H      -2.624642    -4.608473    -1.627879      12.73
 C      -3.511656    -3.189635     0.135449      85.03
 H      -2.554790    -3.611518     0.678354      22.57
 O      -4.233898    -2.330337     0.872005     338.36
 H      -3.960829    -2.210595     1.902759      26.08
 C      -4.366602    -4.533669    -0.114284     104.25
 O      -3.757414    -5.577077    -1.022365     367.60
 H      -3.259784    -6.029667    -0.401462      30.35
 H      -5.133710    -4.157522    -0.715074      26.87
 H      -4.660880    -5.087782     0.736293      27.78
55
name = lig-etoh-frame_963
 C       2.545281     1.578800    -2.226325      80.25
 H       2.003121     2.139957    -2.989307      25.27
 C       3.569556     1.344765     0.004927      64.67
 H       3.960408     1.743778     0.896008      24.84
 C       4.313084     0.178471    -0.410719       6.72
 O       5.174758    -0.391509     0.413757     198.97
 C       4.740356    -0.455485     2.001440      80.65
 H       3.613191    -0.454780     2.109274      26.68
 H       5.060759     0.562351     2.214192      23.17
 H       5.261390    -1.228830     2.424233      26.35
 C       4.115462    -0.379590    -1.795286       9.80
 O       4.590011    -1.689700    -2.349264     159.32
 H       4.805749    -2.163716    -1.334535      21.96
 C       3.332768     0.433961    -2.714971      40.69
 H       2.991123    -0.037591    -3.599176      24.52
 C       2.740214     1.981791    -0.947622      26.52
 C       2.029520     3.280013    -0.513789     115.14
 H       2.260207     4.164052    -0.980597      20.17
 O       2.311988     3.735568     0.885301     331.84
 H       3.259928     3.529614     1.101080      28.08
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 C       0.374509     3.274918    -0.538088      53.74
 H       0.024885     3.069292    -1.611579      20.55
 C      -0.280928     4.599063    -0.195272     101.48
 O       0.466426     5.757728    -0.656868     304.41
 H       0.503676     5.669419    -1.558668      31.92
 H      -0.225654     4.782000     0.880565      24.58
 H      -1.361155     4.589702    -0.511631      24.11
 C      -0.847899    -1.172965    -0.412991      49.33
 H      -0.400709    -2.013523    -0.690244      21.80
 C      -2.900952    -0.020683    -0.822024      52.62
 H      -4.041959    -0.081009    -0.796261      23.07
 C      -2.384424     1.269608    -0.488696     -11.43
 O      -3.014813     2.578768    -0.461607     181.41
 C      -4.376083     2.719656    -0.115832     124.00
 H      -4.968443     2.189370     0.797045      24.70
 H      -4.778545     3.625868    -0.209758      28.65
 H      -4.873435     2.201423    -1.034500      23.44
 C      -0.900082     1.179542    -0.069455      -5.46
 O      -0.219025     2.241931     0.523461     124.37
 C      -0.242937     0.036790    -0.185864      59.91
 H       0.812058    -0.129123     0.051457      21.87
 C      -2.187683    -1.211203    -0.883393      13.90
 C      -2.954770    -2.558948    -1.159922      93.52
 H      -3.938552    -2.544837    -1.587262      23.84
 O      -2.122261    -3.608805    -1.663599     260.47
 H      -2.499424    -4.451695    -1.596009      21.65
 C      -3.430885    -3.233396     0.099751      85.61
 H      -2.550827    -3.462671     0.630962      23.76
 O      -4.256961    -2.273576     0.911966     304.58
 H      -3.951115    -2.317946     2.019507      23.69
 C      -4.340216    -4.536525    -0.168522      81.51
 O      -3.659946    -5.504814    -1.016171     313.04
 H      -3.400326    -6.300194    -0.295679      24.14
 H      -5.327714    -4.369711    -0.829947      23.09
 H      -4.435508    -5.041644     0.861397      25.06
55
name = lig-etoh-frame_964
 C       2.627839     1.554993    -2.267834      63.68
 H       1.990528     2.159633    -2.931369      22.61
 C       3.611681     1.337104    -0.020240      48.17
 H       3.465682     1.890515     1.038720      19.01
 C       4.279866     0.200382    -0.524731       2.36
 O       5.164848    -0.382644     0.451786     207.68
 C       4.758658    -0.470221     1.971501      86.41
 H       3.716566    -0.642848     2.045324      28.39
 H       5.207562     0.432715     2.409325      24.70
 H       5.450773    -1.353208     2.397744      24.64
 C       4.110524    -0.456156    -1.808751      33.17
 O       4.645224    -1.661177    -2.281630     243.70
 H       4.709040    -2.292645    -1.583624      28.37
 C       3.433340     0.394816    -2.728424      50.21
 H       2.936919    -0.041366    -3.701759      24.17
 C       2.665035     1.973260    -0.897360      36.33
 C       2.059318     3.322860    -0.443492      93.15
 H       2.156738     4.408528    -0.973539      16.95
 O       2.304208     3.735453     0.883699     292.22
 H       3.318704     3.633100     1.095866      28.05
 C       0.316409     3.262225    -0.591276      38.98
 H       0.033812     2.589033    -1.417791      20.98
 C      -0.300669     4.624780    -0.214692      97.81
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 O       0.424255     5.789707    -0.624710     254.96
 H       0.544851     5.744800    -1.759067      23.19
 H      -0.227911     4.813587     0.873342      23.26
 H      -1.357415     4.514119    -0.465421      24.18
 C      -0.888554    -1.193170    -0.414632      68.72
 H      -0.278387    -2.253489    -0.519363      21.88
 C      -2.877603    -0.031308    -0.875885      29.16
 H      -3.906147     0.034397    -0.670865      24.72
 C      -2.357736     1.348092    -0.475599     -19.96
 O      -2.982618     2.575714    -0.418136     133.75
 C      -4.389516     2.684893    -0.120814      91.23
 H      -4.418287     2.322447     0.871263      24.90
 H      -4.676626     3.891255    -0.150200      22.55
 H      -4.986504     1.957530    -1.198931      18.43
 C      -0.932608     1.203447    -0.094000      -1.84
 O      -0.263682     2.268494     0.534290     135.26
 C      -0.258430     0.019489    -0.224429      50.09
 H       0.809036     0.034396     0.123277      22.59
 C      -2.200766    -1.225628    -0.815691      20.95
 C      -2.988629    -2.584652    -1.116381      85.17
 H      -3.767182    -2.506419    -2.060051      18.32
 O      -2.116761    -3.556942    -1.659583     210.73
 H      -2.611538    -4.516223    -1.482715      14.69
 C      -3.398322    -3.261741     0.133575      79.33
 H      -2.456200    -3.497340     0.759583      22.19
 O      -4.268740    -2.233098     0.954364     279.10
 H      -4.074828    -2.514962     1.911801      25.93
 C      -4.308301    -4.526050    -0.222767     103.30
 O      -3.560998    -5.460972    -0.989929     318.57
 H      -3.329694    -6.416112    -0.689721      28.58
 H      -5.360055    -4.443083    -0.475830      27.67
 H      -4.455014    -4.777536     0.821234      28.54
55
name = lig-etoh-frame_965
 C       2.737747     1.509813    -2.298913      55.98
 H       2.055606     2.036825    -2.967398      21.32
 C       3.586935     1.357893    -0.075494      66.82
 H       3.392522     1.522113     0.923868      23.24
 C       4.274729     0.193572    -0.551869       7.21
 O       5.152756    -0.402095     0.495036     220.04
 C       4.837063    -0.481552     1.889959     104.95
 H       3.735489    -0.857702     2.062561      27.87
 H       5.099687     0.321806     2.661136      25.36
 H       5.390577    -1.378126     2.169917      26.37
 C       4.097379    -0.474277    -1.820607      32.66
 O       4.695846    -1.620886    -2.214220     242.27
 H       4.710618    -2.383322    -1.602634      28.55
 C       3.444360     0.366471    -2.739877      50.22
 H       3.273123     0.023214    -3.700748      24.92
 C       2.634049     1.999910    -0.870457      60.01
 C       1.998154     3.393474    -0.400266     113.33
 H       2.263419     4.038214    -1.224699      24.09
 O       2.307893     3.721056     0.913153     331.38
 H       3.218878     3.871131     1.020784      32.22
 C       0.316773     3.213144    -0.584024      49.38
 H       0.105800     2.529057    -1.427130      22.72
 C      -0.319994     4.646708    -0.214787      91.65
 O       0.381257     5.827414    -0.642272     278.93
 H       0.482914     5.891428    -1.610372      29.08
 H      -0.294246     4.560213     0.902113      24.51
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 H      -1.415199     4.655532    -0.531591      23.70
 C      -0.887965    -1.286625    -0.460907      81.07
 H      -0.286816    -2.098191    -0.148817      28.40
 C      -2.901982     0.079396    -0.887188      13.07
 H      -4.059349    -0.060164    -0.852389      23.76
 C      -2.282908     1.331797    -0.469733      17.97
 O      -2.922902     2.572208    -0.381083     134.90
 C      -4.395510     2.665156    -0.140113      87.94
 H      -4.248121     2.319173     0.966583      24.05
 H      -4.475954     3.661869    -0.151813      26.99
 H      -5.241955     1.874170    -1.091372      20.42
 C      -1.012717     1.299205    -0.109150       2.50
 O      -0.297473     2.315502     0.522054     164.47
 C      -0.227839    -0.023892    -0.224586      -9.57
 H       0.763639     0.191887     0.097776      23.69
 C      -2.251214    -1.272199    -0.767427     -43.40
 C      -3.004819    -2.576687    -1.117435     116.89
 H      -3.529092    -2.207900    -1.928929      20.64
 O      -2.069800    -3.521961    -1.684060     239.64
 H      -2.487550    -4.389637    -1.480473      16.02
 C      -3.452638    -3.236690     0.197502      89.74
 H      -2.588776    -3.606206     0.745435      24.04
 O      -4.250524    -2.227626     0.969531     216.95
 H      -4.333098    -2.755325     2.011994      23.34
 C      -4.263707    -4.512625    -0.179505      91.66
 O      -3.474352    -5.431948    -1.000707     333.91
 H      -3.217111    -6.278314    -0.720574      31.42
 H      -5.359177    -4.275136    -0.475627      26.35
 H      -4.489433    -4.890458     0.876441      28.25
55
name = lig-etoh-frame_966
 C       2.809178     1.504170    -2.291124      82.38
 H       2.218155     1.891097    -3.148297      20.94
 C       3.527889     1.343899    -0.138795      52.58
 H       3.642148     1.219202     1.054864      20.65
 C       4.289785     0.164424    -0.488984      14.55
 O       5.138484    -0.419988     0.489233     263.00
 C       4.881256    -0.526266     1.826109     113.39
 H       3.892693    -0.846246     2.033816      30.46
 H       4.933905     0.292563     2.518585      26.77
 H       5.490839    -1.489434     2.080971      25.06
 C       4.102145    -0.436504    -1.774405      29.57
 O       4.756994    -1.593255    -2.173916     151.51
 H       4.679257    -2.371597    -1.357194      24.26
 C       3.416466     0.346018    -2.741700      55.31
 H       3.651226     0.072544    -3.879862      27.73
 C       2.652977     2.025852    -0.921688      61.50
 C       1.882917     3.377226    -0.417166     122.03
 H       2.363620     3.898481    -1.352367      21.69
 O       2.303475     3.712986     0.954791     279.90
 H       3.210676     4.168442     0.930690      29.14
 C       0.360518     3.192559    -0.528495      78.89
 H       0.208717     2.901406    -1.611152      23.07
 C      -0.353456     4.641032    -0.231534      94.54
 O       0.337560     5.869721    -0.637194     256.58
 H       0.357523     5.857997    -1.711124      25.38
 H      -0.345075     4.501666     0.843143      25.39
 H      -1.345874     4.791810    -0.594956      24.60
 C      -0.846062    -1.316588    -0.479242      13.29
 H      -0.302851    -2.226562     0.016096      24.30
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 C      -2.949837     0.135861    -0.868799      61.45
 H      -3.940962     0.036585    -1.204107      28.44
 C      -2.304106     1.290118    -0.490018      29.28
 O      -2.872428     2.563291    -0.371034     173.47
 C      -4.342370     2.587779    -0.144335     119.27
 H      -4.684381     2.275520     0.861448      27.87
 H      -4.564265     3.769228    -0.264421      25.77
 H      -5.249956     2.169318    -0.499426      26.51
 C      -0.958093     1.295386    -0.098248       7.58
 O      -0.321449     2.376180     0.492088     180.34
 C      -0.260609    -0.014330    -0.203654       7.75
 H       0.863859     0.106862     0.037427      23.81
 C      -2.309083    -1.250799    -0.738024     -64.27
 C      -2.957987    -2.531098    -1.100703      86.85
 H      -3.893607    -2.065416    -1.786289      21.88
 O      -1.996209    -3.467987    -1.727659     154.55
 H      -2.339827    -4.443631    -1.567085       9.94
 C      -3.559374    -3.188144     0.236715      98.34
 H      -2.621978    -3.571049     0.758496      22.78
 O      -4.230357    -2.274193     0.995490     336.03
 H      -4.400965    -2.527898     1.795882      33.47
 C      -4.253076    -4.512943    -0.056295      87.59
 O      -3.418422    -5.384423    -1.036040     294.23
 H      -3.028718    -6.212566    -0.310543      20.52
 H      -5.046490    -4.161523    -0.790979      23.62
 H      -4.471501    -5.237600     0.750220      26.95
55
name = lig-etoh-frame_967
 C       2.811211     1.544786    -2.315016      64.50
 H       2.386429     2.013018    -3.199322      21.41
 C       3.504281     1.251202    -0.105922      40.33
 H       3.730522     1.538377     0.899982      21.85
 C       4.281070     0.140317    -0.420517      16.27
 O       5.138419    -0.434691     0.410588     273.08
 C       4.895890    -0.617841     1.813608      99.47
 H       3.776486    -0.939229     1.960482      26.88
 H       5.068856     0.437002     2.272341      23.63
 H       5.677242    -1.351632     2.219339      25.33
 C       4.139430    -0.390543    -1.706905      25.53
 O       4.811820    -1.588469    -2.122524     243.21
 H       4.786439    -2.026266    -1.341895      29.55
 C       3.425827     0.306727    -2.734535      63.55
 H       3.761292     0.233231    -3.711760      33.77
 C       2.684502     2.035071    -1.009353      44.22
 C       1.823940     3.286765    -0.456618     118.16
 H       2.131985     4.176016    -1.089101      22.77
 O       2.298806     3.706970     0.971925     240.65
 H       3.003587     4.455651     0.806258      27.83
 C       0.390586     3.261200    -0.500806      93.42
 H       0.183704     3.188723    -1.573598      22.17
 C      -0.363325     4.632657    -0.246817      87.50
 O       0.297954     5.901925    -0.636988     246.60
 H       0.260416     5.763101    -1.694065      26.28
 H      -0.449268     4.781822     0.878770      23.76
 H      -1.422552     4.648835    -0.708709      23.11
 C      -0.846231    -1.267007    -0.453761      32.69
 H      -0.456736    -2.296265    -0.187556      24.19
 C      -2.983207     0.077521    -0.853505      59.25
 H      -3.921848     0.294307    -1.522926      23.54
 C      -2.331717     1.278600    -0.493962      -3.99
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 O      -2.868344     2.534259    -0.376523     146.20
 C      -4.261750     2.610071    -0.074857      87.77
 H      -4.739809     2.323811     0.905144      24.75
 H      -4.650506     3.549497    -0.316783      26.18
 H      -5.553556     1.881092    -0.867171      19.10
 C      -0.860349     1.192139    -0.089588       1.67
 O      -0.331106     2.424588     0.440495     176.76
 C      -0.277188     0.013340    -0.165965      71.23
 H       0.749501    -0.114277    -0.024507      25.08
 C      -2.290381    -1.158990    -0.722340     -27.38
 C      -2.960456    -2.482729    -1.088624      89.55
 H      -3.913107    -2.467814    -1.499651      23.63
 O      -1.934762    -3.381276    -1.776294     153.88
 H      -2.298792    -4.351506    -1.644558      12.48
 C      -3.574590    -3.194484     0.272634      91.88
 H      -2.605352    -3.348675     0.804312      23.47
 O      -4.243652    -2.281643     0.989054     250.70
 H      -4.362839    -2.478619     2.138249      23.69
 C      -4.257150    -4.526412    -0.010030      98.04
 O      -3.365676    -5.365088    -1.018563     381.20
 H      -2.839543    -5.803149    -0.438244      29.40
 H      -4.975869    -4.316843    -0.806518      24.40
 H      -4.609026    -5.304462     0.669704      27.43
55
name = lig-etoh-frame_968
 C       2.784156     1.581754    -2.393335      48.25
 H       2.442242     2.309557    -3.145272      22.96
 C       3.470887     1.204030    -0.039604      69.23
 H       3.606559     1.993928     0.864894      22.38
 C       4.227415     0.129408    -0.386519      35.36
 O       5.180536    -0.489989     0.334813     259.17
 C       4.894335    -0.663742     1.818014     115.23
 H       3.928413    -1.031924     1.953793      29.22
 H       5.137276     0.295991     2.139311      26.08
 H       5.710256    -1.257833     2.279311      26.73
 C       4.184952    -0.374370    -1.708274      16.40
 O       4.853350    -1.556829    -2.069051     188.13
 H       5.095750    -1.988860    -1.113246      20.70
 C       3.461779     0.311600    -2.659457      63.65
 H       3.726080     0.201571    -3.780568      28.17
 C       2.727879     2.015622    -1.055327      78.12
 C       1.879184     3.221771    -0.463458     116.47
 H       1.894242     4.319488    -0.918366      17.08
 O       2.291911     3.696610     0.953310     309.89
 H       2.668477     4.519558     0.783928      31.11
 C       0.354214     3.377589    -0.507468      74.88
 H       0.019455     3.071792    -1.547469      20.23
 C      -0.377303     4.670769    -0.217908     106.54
 O       0.250952     5.904951    -0.662006     276.72
 H       0.358850     5.930881    -1.610879      31.02
 H      -0.596739     4.947602     0.786029      24.79
 H      -1.280351     4.380214    -0.719954      23.75
 C      -0.941752    -1.174722    -0.415297     106.01
 H      -0.483347    -2.165115    -0.471189      26.23
 C      -3.012965     0.044903    -0.862372      43.45
 H      -3.811056     0.269748    -1.496412      22.74
 C      -2.280339     1.235785    -0.459951     -28.24
 O      -2.903593     2.500779    -0.386443     155.84
 C      -4.287326     2.604828    -0.054279     111.41
 H      -4.385915     2.269778     1.076325      23.87
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 H      -4.642527     3.645329    -0.375253      24.28
 H      -4.790837     1.968033    -0.880236      20.14
 C      -0.877068     1.174365    -0.091076      -0.09
 O      -0.333536     2.429778     0.378073     155.00
 C      -0.211400    -0.050638    -0.123592      68.17
 H       0.909033    -0.159069     0.069747      23.73
 C      -2.247972    -1.105507    -0.743276      26.86
 C      -2.966828    -2.476873    -1.047648      83.82
 H      -3.941823    -2.650952    -1.736014      17.55
 O      -1.901886    -3.267547    -1.816319     188.25
 H      -2.345942    -4.118144    -1.719430      17.70
 C      -3.467562    -3.239422     0.321773      80.99
 H      -2.546580    -3.378735     0.913906      23.46
 O      -4.322751    -2.247160     1.026255     322.39
 H      -3.928594    -2.461574     1.903208      26.66
 C      -4.249224    -4.559960    -0.063184      82.08
 O      -3.333705    -5.326050    -0.985472     353.66
 H      -2.473923    -5.829480    -0.451347      21.89
 H      -5.284688    -4.449869    -0.651070      23.90
 H      -4.746106    -5.135619     0.812990      25.99
55
name = lig-etoh-frame_969
 C       2.768246     1.603624    -2.443985      22.80
 H       2.418222     2.332630    -3.152679      23.76
 C       3.402980     1.262188     0.024875      74.54
 H       3.482443     2.002502     0.833981      24.13
 C       4.175142     0.114985    -0.372349      32.46
 O       5.241615    -0.584457     0.307395     226.15
 C       4.930630    -0.674437     1.783071      99.73
 H       3.903736    -1.148106     2.041038      26.27
 H       4.977501     0.385563     2.302603      23.40
 H       5.766163    -1.420679     2.235021      24.99
 C       4.215975    -0.381461    -1.730749       9.21
 O       4.883068    -1.525026    -1.992017     181.54
 H       5.604994    -1.788492    -1.227367      19.65
 C       3.495967     0.385622    -2.644706      59.88
 H       3.517318    -0.056604    -3.657476      23.14
 C       2.759114     1.978067    -1.051741      70.42
 C       1.956186     3.243320    -0.452656     109.67
 H       2.111931     4.145433    -1.117940      18.20
 O       2.282138     3.657188     0.916340     308.45
 H       2.442528     4.658716     0.838250      28.17
 C       0.309028     3.406307    -0.543211      61.25
 H       0.003049     3.003117    -1.501381      20.60
 C      -0.394900     4.739381    -0.195449      94.91
 O       0.200647     5.908643    -0.685635     263.95
 H       0.521996     6.028437    -1.747357      24.48
 H      -0.702356     4.880968     0.902118      22.58
 H      -1.355373     4.413509    -0.739382      21.05
 C      -1.002143    -1.116485    -0.360740      65.53
 H      -0.396804    -2.060453    -0.767018      23.28
 C      -2.985146     0.084959    -0.860174      68.80
 H      -4.017950     0.032642    -1.398642      20.39
 C      -2.247236     1.189378    -0.416934      20.42
 O      -2.895194     2.478594    -0.400466     191.21
 C      -4.317850     2.606901    -0.031809     112.88
 H      -4.312869     2.288649     0.959714      26.79
 H      -4.523035     3.690772    -0.179617      25.33
 H      -4.364293     1.682570    -0.969834      16.31
 C      -0.919970     1.225278    -0.088499     -22.21
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 O      -0.341097     2.396820     0.336713     163.00
 C      -0.103123    -0.099921    -0.069871      19.00
 H       0.929679    -0.075149     0.171756      22.11
 C      -2.314516    -1.122923    -0.806798      17.98
 C      -2.963133    -2.502573    -1.020006     107.92
 H      -3.650329    -2.357868    -1.798291      24.02
 O      -1.892415    -3.144372    -1.837338     164.43
 H      -2.358347    -4.119789    -1.921182      15.46
 C      -3.370482    -3.254345     0.329859      73.99
 H      -2.540746    -3.617728     1.037564      22.15
 O      -4.377407    -2.235092     1.046429     275.39
 H      -3.848339    -2.290486     1.997739      23.55
 C      -4.245238    -4.595579    -0.117517      93.76
 O      -3.308636    -5.283271    -0.943410     362.19
 H      -2.691350    -5.954642    -0.455694      24.38
 H      -5.179836    -4.380369    -0.551784      27.23
 H      -4.475571    -4.969438     0.873935      28.03
55
name = lig-etoh-frame_970
 C       2.780540     1.604874    -2.409390      50.65
 H       2.284264     2.094740    -3.263234      22.00
 C       3.360327     1.307564     0.032037      56.79
 H       3.469201     1.773483     1.113234      20.58
 C       4.162469     0.103047    -0.362970      15.16
 O       5.263355    -0.664904     0.332241     230.17
 C       4.986899    -0.683892     1.757184     128.02
 H       4.048627    -1.151793     1.939727      29.99
 H       4.861259     0.208572     2.284781      27.66
 H       5.683343    -1.375022     2.102468      27.60
 C       4.212188    -0.346966    -1.693610      24.96
 O       4.936949    -1.509076    -1.937290     220.64
 H       5.695588    -1.460609    -1.458762      27.59
 C       3.516675     0.446514    -2.705033      61.15
 H       3.352561    -0.173219    -3.610535      25.30
 C       2.741705     1.969619    -1.013790      33.73
 C       1.996690     3.309828    -0.477047     112.05
 H       2.538833     3.998801    -1.362869      18.55
 O       2.287271     3.616256     0.868063     298.62
 H       2.202033     4.637357     1.024192      26.50
 C       0.299532     3.349190    -0.581604      60.63
 H       0.063080     3.147399    -1.667080      20.08
 C      -0.449635     4.771918    -0.203496      95.36
 O       0.175461     5.949363    -0.713341     307.19
 H       0.366462     5.710557    -1.610085      29.34
 H      -0.557236     4.769967     0.861574      24.16
 H      -1.452258     4.790727    -0.622180      23.03
 C      -0.956518    -1.131209    -0.340304      51.70
 H      -0.493529    -1.990729    -0.613517      24.98
 C      -2.973342     0.099230    -0.879179      69.16
 H      -4.046867    -0.039739    -0.976186      26.84
 C      -2.288301     1.212690    -0.389015       0.80
 O      -2.825299     2.480604    -0.406884     158.90
 C      -4.291409     2.558230    -0.068195      95.15
 H      -4.595348     2.170003     1.102441      24.18
 H      -4.571001     3.623115    -0.087419      25.99
 H      -4.963597     1.790911    -0.723554      23.10
 C      -0.871284     1.218174    -0.071391     -21.46
 O      -0.341983     2.371506     0.332370     174.12
 C      -0.102784    -0.039870    -0.020121      48.40
 H       1.000239    -0.089627     0.223555      22.75
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 C      -2.400806    -1.147220    -0.839287     -31.22
 C      -2.906012    -2.496586    -1.004722     100.93
 H      -3.827724    -2.134078    -1.688515      21.73
 O      -1.906051    -3.070364    -1.854619     222.87
 H      -2.092917    -3.935202    -2.108527      24.54
 C      -3.365754    -3.247495     0.300710      78.98
 H      -2.616622    -3.644515     0.935589      22.58
 O      -4.369384    -2.266055     1.046410     265.70
 H      -4.240854    -2.034392     2.102202      25.38
 C      -4.183498    -4.573504    -0.104927      73.55
 O      -3.300259    -5.263753    -0.929093     309.99
 H      -2.994058    -6.119661    -0.319905      22.59
 H      -5.161354    -4.211488    -0.720895      23.45
 H      -4.179727    -5.104929     0.910034      25.32
55
name = lig-etoh-frame_971
 C       2.803077     1.584459    -2.344432      67.38
 H       2.096503     1.862949    -3.148484      20.73
 C       3.393682     1.287006     0.034314      62.13
 H       3.338707     1.325895     1.173814      19.13
 C       4.192165     0.107472    -0.344841      16.02
 O       5.230724    -0.693888     0.369933     216.88
 C       5.024633    -0.718107     1.727359     108.31
 H       4.021995    -1.266151     1.832270      27.34
 H       5.014087     0.326983     2.257556      24.83
 H       5.927123    -1.429111     2.254053      24.09
 C       4.184011    -0.281478    -1.660402      26.33
 O       4.970273    -1.491044    -1.921732     139.43
 H       5.956951    -1.166839    -1.511014      23.39
 C       3.540084     0.445886    -2.753124      43.75
 H       3.261945    -0.070792    -3.746734      24.82
 C       2.673405     2.011128    -0.950179      40.45
 C       1.998353     3.380374    -0.560310     118.37
 H       2.660854     3.945421    -1.212119      22.50
 O       2.304809     3.587204     0.829151     349.05
 H       2.039837     4.420317     1.107473      31.71
 C       0.308695     3.311421    -0.649917      64.79
 H       0.080016     3.203447    -1.710980      21.05
 C      -0.497341     4.765886    -0.220348      77.38
 O       0.162628     5.984868    -0.714614     250.87
 H       0.277659     5.647792    -1.716964      25.21
 H      -0.330592     4.778893     0.916137      22.42
 H      -1.580627     4.930796    -0.498201      22.29
 C      -0.913904    -1.150973    -0.358040      13.27
 H      -0.420070    -2.292919    -0.234164      23.64
 C      -3.005707     0.085018    -0.874977      68.08
 H      -4.114017     0.182107    -0.710106      26.93
 C      -2.294414     1.250831    -0.379585     -16.86
 O      -2.799158     2.498368    -0.400237     126.97
 C      -4.273859     2.465414    -0.089725     128.82
 H      -4.542001     2.169998     0.865026      29.04
 H      -4.592451     3.575743    -0.099648      25.98
 H      -5.445418     2.365215    -0.346606      22.01
 C      -0.831644     1.158576    -0.061775      17.27
 O      -0.309216     2.389104     0.347359     163.10
 C      -0.181451     0.037788     0.013433      91.69
 H       0.868243    -0.116969     0.202172      24.77
 C      -2.330317    -1.126575    -0.783025     -17.75
 C      -2.913905    -2.458400    -1.029599     110.44
 H      -3.942826    -2.416433    -1.340861      26.21
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 O      -1.911837    -3.017667    -1.881435     202.47
 H      -2.017651    -3.970689    -2.165849      21.77
 C      -3.432305    -3.217652     0.281307      90.23
 H      -2.468633    -3.468644     0.909184      23.80
 O      -4.348964    -2.305546     1.004769     324.13
 H      -4.264373    -2.309406     1.905551      31.89
 C      -4.115845    -4.484585    -0.054764     112.81
 O      -3.271509    -5.288786    -0.934526     261.98
 H      -3.332059    -6.256816    -0.448302      23.95
 H      -4.983971    -4.301219    -0.566362      27.66
 H      -4.331382    -5.172817     0.744877      27.10
55
name = lig-etoh-frame_972
 C       2.798301     1.548538    -2.272712      62.66
 H       1.974584     1.919038    -2.891954      20.19
 C       3.450082     1.203485     0.049685      85.63
 H       3.240858     1.319472     1.079458      21.56
 C       4.242208     0.133509    -0.322658      13.66
 O       5.169418    -0.675931     0.370319     244.41
 C       5.061118    -0.771063     1.772160     144.03
 H       4.130411    -1.256926     2.039014      30.04
 H       5.188465     0.215610     2.111708      28.96
 H       5.824247    -1.257371     2.171431      29.10
 C       4.185961    -0.259659    -1.700053      25.75
 O       5.002846    -1.435405    -1.921192     193.41
 H       5.928785    -1.218953    -1.636256      26.73
 C       3.544686     0.419996    -2.743340      32.88
 H       3.414333     0.142758    -3.748043      25.60
 C       2.619618     2.036284    -0.895474     104.18
 C       1.960081     3.397233    -0.607809     116.99
 H       2.488204     4.335623    -1.240374      23.88
 O       2.331486     3.553162     0.792916     315.81
 H       1.873263     4.387998     1.158784      29.19
 C       0.312452     3.346558    -0.722433      66.21
 H      -0.029722     2.974903    -1.729122      23.01
 C      -0.494064     4.754072    -0.213967      87.22
 O       0.146977     5.979961    -0.719768     245.76
 H       0.319945     6.142858    -1.739009      27.72
 H      -0.273755     4.821580     0.826223      25.58
 H      -1.568088     4.649035    -0.371839      24.58
 C      -0.883339    -1.204769    -0.370062     100.15
 H      -0.500185    -2.011356     0.039697      29.23
 C      -3.027483     0.112517    -0.807982      66.09
 H      -4.132512     0.315853    -0.741901      26.31
 C      -2.242126     1.231228    -0.408026      -4.19
 O      -2.836529     2.514287    -0.397542     103.04
 C      -4.318996     2.479350    -0.082962     106.47
 H      -4.160574     2.022749     1.104122      23.78
 H      -4.299391     3.568625     0.033511      26.00
 H      -5.268900     2.316091    -0.724445      23.69
 C      -0.893695     1.213625    -0.066058      15.62
 O      -0.243698     2.422122     0.355360     169.43
 C      -0.244244    -0.020980     0.024587      53.98
 H       0.819375    -0.013039     0.273319      24.63
 C      -2.195285    -1.097677    -0.687282     -15.22
 C      -2.974974    -2.426007    -1.037515      88.79
 H      -4.014473    -2.533367    -1.544250      23.91
 O      -1.920462    -2.996548    -1.924223     151.69
 H      -2.168933    -4.031355    -1.974290      17.73
 C      -3.424455    -3.164216     0.312646     113.37
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 H      -2.548510    -3.219054     0.873243      26.01
 O      -4.330609    -2.344423     0.916613     248.22
 H      -4.038820    -2.819782     1.979330      20.53
 C      -4.054863    -4.436907    -0.014141      92.20
 O      -3.259809    -5.333894    -0.953869     292.00
 H      -3.266849    -6.176263    -0.718190      30.67
 H      -5.159422    -4.282179    -0.550312      24.74
 H      -4.581233    -5.063225     0.797043      26.71
55
name = lig-etoh-frame_973
 C       2.734617     1.532915    -2.182065      30.61
 H       2.054883     2.111738    -2.848301      20.23
 C       3.456476     1.161556     0.076187      85.97
 H       3.277750     1.607957     1.199823      22.05
 C       4.290734     0.151316    -0.343803      21.14
 O       5.100985    -0.652151     0.350938     227.29
 C       5.068507    -0.786845     1.826393      94.99
 H       4.161587    -1.214504     2.359407      27.17
 H       5.178484     0.295401     2.211671      24.22
 H       6.122272    -1.492934     2.102389      22.95
 C       4.257012    -0.285302    -1.750996      35.41
 O       5.014894    -1.371057    -1.956809     203.04
 H       5.886118    -1.316761    -1.631381      27.62
 C       3.517688     0.417953    -2.674243      61.98
 H       3.711084     0.252931    -3.841661      27.28
 C       2.647202     1.989601    -0.894689      69.55
 C       1.914766     3.401593    -0.625467     109.71
 H       1.939999     4.351399    -1.150957      22.11
 O       2.347188     3.539244     0.762232     351.19
 H       1.807797     4.315983     1.166431      28.24
 C       0.298941     3.410768    -0.768765      68.13
 H      -0.087725     2.844613    -1.621961      22.63
 C      -0.423073     4.722517    -0.251491      93.20
 O       0.119875     5.984200    -0.715880     255.14
 H       0.238634     6.152848    -1.631509      32.15
 H      -0.282460     4.823204     0.880353      23.91
 H      -1.492826     4.370382    -0.370788      22.50
 C      -0.844078    -1.221681    -0.343841      84.39
 H      -0.387653    -2.224769     0.199404      24.94
 C      -2.964848     0.132753    -0.694201      84.31
 H      -4.011044     0.122752    -0.955517      24.76
 C      -2.237549     1.251003    -0.465099      27.84
 O      -2.889467     2.508625    -0.414973     200.15
 C      -4.336386     2.543998    -0.012505     122.25
 H      -4.316120     1.940821     0.772708      28.64
 H      -4.275711     3.643185     0.310768      24.21
 H      -4.569541     1.991170    -1.056135      20.90
 C      -0.927347     1.299761    -0.061925      -6.39
 O      -0.172472     2.439440     0.351925     139.67
 C      -0.264461    -0.066226     0.027195      -2.57
 H       0.762508     0.075914     0.422322      24.18
 C      -2.224736    -1.084660    -0.637334     -24.56
 C      -3.019201    -2.388317    -1.045951      99.47
 H      -3.746597    -2.198533    -1.847464      23.69
 O      -1.963811    -3.027307    -1.951523     225.59
 H      -2.218072    -3.897391    -1.811423      21.39
 C      -3.330594    -3.113297     0.277540      95.57
 H      -2.392177    -3.168847     1.004314      22.72
 O      -4.325797    -2.386147     0.902741     300.20
 H      -4.265099    -2.621458     1.771052      30.80
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 C      -4.077855    -4.490376    -0.021631      92.33
 O      -3.270754    -5.326895    -0.982241     234.69
 H      -3.079470    -6.405645    -0.685628      22.43
 H      -4.874656    -4.106269    -0.539948      28.11
 H      -4.402217    -4.867363     0.935276      29.05
55
name = lig-etoh-frame_974
 C       2.645065     1.521206    -2.157020      62.34
 H       2.325845     2.186628    -2.958660      25.46
 C       3.412690     1.209143     0.131473      63.31
 H       3.560736     1.602362     1.038572      27.58
 C       4.290817     0.175846    -0.398607      21.68
 O       5.050556    -0.662220     0.374277     228.98
 C       5.119814    -0.777256     1.882270     119.39
 H       4.219842    -1.226547     2.331095      28.94
 H       5.193392     0.179633     2.345121      27.09
 H       5.850745    -1.384359     1.916596      28.53
 C       4.336783    -0.272576    -1.746989      21.92
 O       5.030199    -1.340873    -2.050498     151.31
 H       5.934587    -1.471495    -1.372361      22.06
 C       3.486834     0.438731    -2.627550      66.95
 H       3.794479     0.331804    -3.584889      27.85
 C       2.710647     1.932608    -0.888832      33.70
 C       1.838941     3.355436    -0.599048      91.20
 H       2.044321     4.341608    -1.336865      19.18
 O       2.340418     3.554166     0.736701     382.39
 H       1.904619     4.231921     1.170482      31.33
 C       0.303555     3.422793    -0.744108      78.83
 H      -0.065194     3.028621    -1.713504      21.97
 C      -0.337808     4.671983    -0.291385     102.78
 O       0.076326     5.992799    -0.692821     249.60
 H       0.124688     5.810426    -1.796954      24.50
 H      -0.276337     4.704877     0.784566      24.94
 H      -1.401449     4.488262    -0.506464      23.15
 C      -0.829279    -1.265400    -0.259367      43.29
 H      -0.418432    -2.202612    -0.146431      25.62
 C      -2.879441     0.084638    -0.590237      66.94
 H      -3.852994    -0.101586    -1.204066      22.81
 C      -2.268462     1.372990    -0.495283      20.03
 O      -2.907444     2.518206    -0.430701     200.76
 C      -4.284163     2.599802    -0.000525     111.34
 H      -4.829831     1.594220     0.735141      22.43
 H      -4.713848     3.555511     0.333181      25.00
 H      -4.550949     2.163863    -0.892411      23.22
 C      -0.874749     1.317482    -0.050660      -4.23
 O      -0.123606     2.432960     0.344579     120.21
 C      -0.247219     0.018818     0.044138      39.64
 H       0.717943    -0.002506     0.534642      24.05
 C      -2.319974    -1.110690    -0.624782       3.34
 C      -2.976438    -2.308184    -1.079047      91.93
 H      -3.718409    -1.843075    -1.781622      24.85
 O      -2.029678    -3.072609    -1.955538     191.32
 H      -2.191225    -4.104812    -1.752894      16.22
 C      -3.220315    -3.121196     0.211308      89.76
 H      -2.382854    -3.224085     0.808704      24.90
 O      -4.354157    -2.390671     0.894773     231.29
 H      -4.432277    -2.386400     2.028970      23.75
 C      -4.051954    -4.541308    -0.045165      76.27
 O      -3.299368    -5.337792    -1.004734     301.46
 H      -2.884710    -6.059558    -0.425772      25.13
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 H      -4.899202    -4.002523    -0.686688      23.07
 H      -4.136543    -4.922044     1.015005      26.76
55
name = lig-etoh-frame_975
 C       2.601514     1.477220    -2.224898      42.19
 H       2.427960     2.208588    -3.027520      24.36
 C       3.397908     1.247791     0.124514      64.42
 H       3.850833     1.643430     1.199702      22.49
 C       4.248036     0.208995    -0.397451      25.39
 O       5.019564    -0.687573     0.429677     222.96
 C       5.118594    -0.733362     1.890629      90.26
 H       4.197349    -1.308636     2.146415      26.21
 H       5.344311     0.219685     2.446692      24.01
 H       6.095147    -1.602863     1.963989      22.92
 C       4.353838    -0.192501    -1.710868      15.32
 O       5.100168    -1.353682    -2.162004     221.57
 H       5.482739    -1.606507    -1.344463      25.31
 C       3.473837     0.465803    -2.569819      47.96
 H       3.691993     0.338133    -3.745154      22.48
 C       2.707022     1.943953    -0.838939      31.09
 C       1.818996     3.314592    -0.588117     116.08
 H       2.477819     3.794206    -1.291298      21.87
 O       2.325459     3.581595     0.717484     342.47
 H       1.945401     4.380193     1.229177      27.71
 C       0.349940     3.354252    -0.700105      95.33
 H       0.066840     3.279338    -1.780327      21.59
 C      -0.307308     4.655337    -0.288795      98.54
 O       0.033205     5.973550    -0.720426     307.75
 H       0.184410     5.849835    -1.640789      31.87
 H      -0.251473     4.582857     0.827688      24.64
 H      -1.368200     4.696385    -0.631642      22.38
 C      -0.898583    -1.220918    -0.176405      30.39
 H      -0.300973    -2.251685    -0.434351      22.54
 C      -2.866680     0.085671    -0.559269      11.86
 H      -3.741786     0.080275    -1.123504      20.61
 C      -2.236002     1.426004    -0.465166       3.74
 O      -2.915257     2.597979    -0.419347     197.14
 C      -4.290445     2.559896     0.001907     121.01
 H      -4.715464     1.878807     0.520001      28.05
 H      -4.924086     3.460558     0.250675      24.46
 H      -5.260528     2.546835    -0.946829      22.31
 C      -0.833466     1.309822    -0.056244      17.97
 O      -0.100267     2.414941     0.333627     165.06
 C      -0.221059     0.081301     0.071872      35.24
 H       0.780734    -0.021177     0.527782      23.60
 C      -2.232531    -1.165857    -0.581865      24.74
 C      -2.917285    -2.262760    -1.137416      95.29
 H      -3.939424    -1.936723    -1.477900      25.00
 O      -2.104445    -3.130130    -1.954087     212.78
 H      -2.219615    -4.101847    -1.740664      19.38
 C      -3.230031    -3.162520     0.152003      70.24
 H      -2.179113    -3.279621     0.697722      23.16
 O      -4.384615    -2.386929     0.894034     243.69
 H      -4.095732    -2.266934     1.944067      24.80
 C      -3.980227    -4.502049    -0.096498     104.04
 O      -3.322110    -5.367603    -1.009268     335.23
 H      -2.724097    -5.862945    -0.329529      25.70
 H      -4.972138    -4.355186    -0.453034      26.37
 H      -4.092451    -5.102196     0.804036      27.46
55
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name = lig-etoh-frame_976
 C       2.601407     1.464886    -2.252196      49.26
 H       2.213123     2.141238    -3.018432      23.53
 C       3.453167     1.276962     0.128895      46.91
 H       3.662870     1.628247     1.044954      22.97
 C       4.221732     0.204032    -0.318247      36.64
 O       4.999263    -0.695329     0.469245     241.82
 C       5.137575    -0.745515     1.868785     137.33
 H       4.206995    -1.255751     2.218133      28.49
 H       5.321762     0.226089     2.321527      27.39
 H       5.874893    -1.305812     2.133390      29.87
 C       4.348006    -0.146534    -1.705853      24.77
 O       5.147445    -1.336828    -2.256822     172.94
 H       5.239285    -1.859112    -1.338484      22.17
 C       3.492392     0.480716    -2.601117      54.91
 H       3.436607     0.235709    -3.598969      22.69
 C       2.605276     1.973705    -0.831723      56.46
 C       1.924399     3.237965    -0.565869     121.48
 H       2.610470     3.723254    -1.375870      18.61
 O       2.307126     3.626974     0.737659     309.69
 H       2.008612     4.566302     1.037259      27.26
 C       0.407061     3.295426    -0.690723      92.59
 H       0.143027     3.125481    -1.736081      21.55
 C      -0.339331     4.665182    -0.241964      90.60
 O       0.018526     5.952502    -0.741373     291.74
 H       0.356126     6.043648    -1.824167      24.22
 H      -0.312986     4.673218     0.867934      24.26
 H      -1.390334     4.503548    -0.572866      22.24
 C      -0.904568    -1.145725    -0.102332     105.88
 H      -0.258563    -1.898144    -0.475829      25.02
 C      -2.860133     0.162306    -0.575136     -18.26
 H      -3.967263     0.349049    -0.947297      19.42
 C      -2.183762     1.361413    -0.390940      -7.34
 O      -2.944427     2.704656    -0.398888     100.65
 C      -4.402205     2.567017    -0.100547      90.74
 H      -4.487059     1.522635     0.820531      21.66
 H      -4.471743     3.592659     0.425877      24.11
 H      -5.184370     2.669612    -0.766103      25.57
 C      -0.825088     1.316264    -0.068157       7.21
 O      -0.090579     2.398406     0.319139     212.76
 C      -0.198280     0.055302     0.109484      41.07
 H       0.862312     0.110437     0.370652      24.04
 C      -2.104131    -1.139901    -0.541994     -10.83
 C      -2.913193    -2.326243    -1.147915     111.21
 H      -3.941534    -2.190823    -1.405444      23.49
 O      -2.166880    -3.171234    -1.980685     242.20
 H      -2.449150    -4.072398    -1.720806      20.11
 C      -3.300543    -3.182863     0.120436      96.61
 H      -2.380778    -3.309541     0.609222      26.01
 O      -4.359320    -2.393045     0.887774     301.68
 H      -3.868422    -2.382461     1.780142      26.69
 C      -3.926603    -4.459352    -0.131232     111.85
 O      -3.321140    -5.420817    -1.024458     296.68
 H      -2.456182    -5.886887    -0.442837      23.31
 H      -5.081802    -4.542522    -0.302363      24.98
 H      -4.074740    -5.113761     0.766331      26.45
55
name = lig-etoh-frame_977
 C       2.603701     1.514596    -2.201530      43.15
 H       1.860298     1.916058    -2.946676      21.69
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 C       3.483038     1.315035     0.090012      66.18
 H       3.406764     1.762226     1.216261      18.62
 C       4.238028     0.149092    -0.247126      25.64
 O       4.992261    -0.700577     0.468426     242.53
 C       5.094420    -0.729062     1.858248     117.76
 H       4.219740    -1.100950     2.447723      29.51
 H       5.154974     0.334224     2.186167      27.65
 H       6.111254    -1.384442     2.270134      25.06
 C       4.349995    -0.163027    -1.717734      13.59
 O       5.163108    -1.272233    -2.296362     166.43
 H       5.065880    -2.157799    -1.659630      23.47
 C       3.509670     0.486730    -2.656789      35.48
 H       3.358775    -0.013636    -3.704538      23.54
 C       2.534461     1.903411    -0.871032      75.49
 C       2.068389     3.217259    -0.551771     113.97
 H       2.249228     4.055639    -1.292558      22.35
 O       2.298143     3.690724     0.790213     312.81
 H       2.097321     4.589046     0.681575      30.27
 C       0.459483     3.293508    -0.697256      66.08
 H       0.100815     2.784045    -1.648615      22.11
 C      -0.385728     4.655971    -0.217881      84.74
 O       0.027208     5.946959    -0.766839     283.65
 H       0.327792     5.870359    -1.705657      28.18
 H      -0.345958     4.852312     0.868339      22.39
 H      -1.393326     4.225098    -0.405827      20.82
 C      -0.779655    -1.078965    -0.036068      12.27
 H      -0.097593    -1.968608    -0.266336      20.59
 C      -2.865414     0.218981    -0.618140      68.99
 H      -3.892625     0.281199    -0.660838      27.56
 C      -2.184840     1.338908    -0.311634      -3.87
 O      -2.957943     2.753002    -0.393051      86.81
 C      -4.457608     2.589717    -0.077390     110.56
 H      -4.418297     1.850168     0.496861      28.83
 H      -4.177379     3.384566     0.617247      22.57
 H      -5.223223     2.509209    -1.150585      22.02
 C      -0.801005     1.296956    -0.056333       5.96
 O      -0.082369     2.386989     0.312304     180.73
 C      -0.167574     0.069218     0.154818      68.57
 H       0.913602     0.163515     0.201536      23.52
 C      -2.181101    -1.049163    -0.579864     -43.46
 C      -2.925155    -2.407398    -1.079370      87.12
 H      -3.867053    -2.078837    -1.710935      20.70
 O      -2.207639    -3.211934    -2.031473     216.11
 H      -2.694534    -4.164181    -1.888972      18.74
 C      -3.386440    -3.147324     0.098025     104.39
 H      -2.462974    -3.356847     0.815100      20.33
 O      -4.297114    -2.409486     0.869194     297.79
 H      -3.790434    -2.577258     1.939346      19.23
 C      -3.959116    -4.525535    -0.124614      96.70
 O      -3.276755    -5.479185    -1.056712     348.41
 H      -2.647067    -5.920296    -0.679346      33.80
 H      -4.992500    -4.384566    -0.478469      26.68
 H      -3.872363    -4.873083     0.935657      27.78
55
name = lig-etoh-frame_978
 C       2.599040     1.533982    -2.203548      60.20
 H       1.686848     1.683883    -2.767484      23.31
 C       3.487627     1.334121     0.068592      68.99
 H       3.249713     1.706957     1.038540      21.52
 C       4.250499     0.115122    -0.257537      13.64
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 O       5.002109    -0.740433     0.457284     226.98
 C       5.065560    -0.682287     1.909198     127.62
 H       4.171854    -1.074893     2.453918      29.20
 H       5.140623     0.394961     2.148755      27.71
 H       5.942046    -1.185965     2.057853      27.95
 C       4.343487    -0.212133    -1.732505      12.15
 O       5.147109    -1.197350    -2.305255     260.68
 H       5.037312    -2.017602    -2.023123      31.61
 C       3.506303     0.485056    -2.695308      28.21
 H       3.436882    -0.075590    -3.620454      24.74
 C       2.574030     1.803267    -0.885672      77.62
 C       2.094349     3.291979    -0.543864     103.23
 H       2.224089     4.188105    -1.170340      21.88
 O       2.303873     3.754257     0.845748     279.15
 H       2.234885     4.724591     0.516017      25.95
 C       0.487072     3.299524    -0.686593      67.26
 H       0.132720     2.813743    -1.584728      23.50
 C      -0.400168     4.624803    -0.220887      79.36
 O       0.021565     5.923873    -0.765950     240.33
 H       0.260690     5.696306    -1.839826      22.57
 H      -0.247296     4.852027     0.875427      21.25
 H      -1.458691     4.264826    -0.361427      20.67
 C      -0.720766    -1.099719    -0.053864     -19.66
 H      -0.198972    -2.102824     0.220033      21.63
 C      -2.874122     0.203115    -0.655354      52.97
 H      -4.027889     0.093757    -0.597191      23.29
 C      -2.203417     1.427162    -0.247561       2.63
 O      -2.937668     2.725707    -0.400319     129.86
 C      -4.445632     2.662608    -0.095591      83.92
 H      -4.679425     1.412455     0.547798      21.61
 H      -4.687508     3.473797     0.754677      23.35
 H      -4.946416     2.542437    -0.900236      27.24
 C      -0.796245     1.297071    -0.018615      16.59
 O      -0.063824     2.388314     0.333467     155.00
 C      -0.088259     0.143765     0.194808      56.76
 H       1.016843     0.144741     0.204147      21.80
 C      -2.249435    -0.995783    -0.623094     -34.58
 C      -2.956898    -2.398781    -1.054603      90.78
 H      -3.606914    -1.904611    -1.720693      22.64
 O      -2.240191    -3.266527    -2.077991     257.18
 H      -2.620980    -4.099774    -2.163977      24.60
 C      -3.400872    -3.143602     0.114655     115.79
 H      -2.566240    -3.336425     0.739337      22.70
 O      -4.237935    -2.420332     0.901058     346.01
 H      -4.136689    -2.562276     1.832918      29.01
 C      -4.003106    -4.627823    -0.103676      87.04
 O      -3.264833    -5.504634    -1.106047     275.91
 H      -2.571979    -6.225218    -0.514730      22.70
 H      -4.971852    -4.384991    -0.638815      25.43
 H      -3.927323    -4.889707     0.938539      28.43
55
name = lig-etoh-frame_979
 C       2.599466     1.462458    -2.287377      61.99
 H       1.640644     1.704167    -2.786463      24.18
 C       3.503926     1.265231     0.048020      61.67
 H       3.357419     1.665697     1.108128      20.48
 C       4.250261     0.112088    -0.346020      19.38
 O       5.011830    -0.796079     0.454901     209.57
 C       5.014035    -0.589332     1.942690     109.10
 H       4.140105    -1.147688     2.314801      27.43
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 H       5.214556     0.429685     2.255410      26.40
 H       6.071026    -1.217371     2.134761      24.66
 C       4.294657    -0.230052    -1.740126      29.04
 O       5.137370    -1.102700    -2.319962     203.99
 H       4.968618    -2.159012    -2.087196      24.43
 C       3.493924     0.478689    -2.665760      34.66
 H       3.489949     0.044464    -3.695816      23.30
 C       2.659821     1.827808    -0.857322      64.84
 C       2.008830     3.361999    -0.524356     103.52
 H       2.656950     4.043799    -1.251892      23.85
 O       2.318096     3.826561     0.874592     263.24
 H       2.497495     4.844959     0.866587      26.83
 C       0.478640     3.317612    -0.644381      84.56
 H       0.212680     3.086352    -1.731676      24.00
 C      -0.373040     4.591304    -0.225004      96.17
 O       0.009940     5.871423    -0.783014     276.41
 H       0.120414     5.852222    -1.815938      26.07
 H      -0.160126     4.610027     0.830814      24.18
 H      -1.440085     4.518448    -0.434686      23.41
 C      -0.752973    -1.113754    -0.098401      26.81
 H      -0.470919    -2.036022     0.399370      23.97
 C      -2.909096     0.204711    -0.662330      26.78
 H      -3.962998     0.053682    -0.820178      26.01
 C      -2.248775     1.506584    -0.221553       9.71
 O      -2.918748     2.665189    -0.389289     186.80
 C      -4.382967     2.665873    -0.006813     103.30
 H      -4.793722     1.807320     0.297036      28.17
 H      -5.087789     3.403069     0.440651      25.59
 H      -5.041553     2.729530    -1.195231      23.25
 C      -0.827090     1.359556     0.032089       7.46
 O      -0.027888     2.413892     0.382427     159.35
 C      -0.020045     0.127478     0.197967      30.04
 H       1.041449     0.211825     0.427836      22.31
 C      -2.174192    -1.049429    -0.628915     -21.04
 C      -2.963622    -2.325219    -1.100296      72.06
 H      -3.884372    -1.840492    -1.660933      22.80
 O      -2.245060    -3.276335    -2.110608     178.93
 H      -2.683866    -4.210646    -2.213260      20.17
 C      -3.372141    -3.221589     0.152177      80.22
 H      -2.299987    -3.387164     0.640156      22.55
 O      -4.233143    -2.389570     0.928843     219.96
 H      -4.396767    -2.669178     2.057155      23.26
 C      -4.025104    -4.691208    -0.122221      88.92
 O      -3.246128    -5.540954    -1.113822     302.81
 H      -2.906010    -6.229388    -0.471510      25.80
 H      -5.071799    -4.626247    -0.601764      25.83
 H      -4.261814    -5.293911     0.846503      27.16
55
name = lig-etoh-frame_980
 C       2.574433     1.398598    -2.305263      66.44
 H       1.845864     1.852737    -3.003216      24.20
 C       3.519678     1.163215     0.057830      65.41
 H       3.761826     1.549694     1.126297      21.57
 C       4.271632     0.082319    -0.426674      14.32
 O       5.007403    -0.820767     0.452930     215.48
 C       5.010961    -0.536269     1.932989     110.91
 H       4.113323    -1.107710     2.285591      26.59
 H       5.121985     0.499553     2.343303      24.34
 H       5.815717    -1.118588     2.399913      26.30
 C       4.225196    -0.213407    -1.741360      42.57
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 O       5.149831    -1.057162    -2.344038     232.41
 H       4.955126    -2.016687    -2.010178      27.51
 C       3.465141     0.449874    -2.651409      41.27
 H       3.575287     0.279552    -3.773723      19.80
 C       2.714342     1.947648    -0.877370      38.18
 C       1.962336     3.414796    -0.491356      97.65
 H       2.631257     3.773843    -1.200650      23.27
 O       2.338515     3.894910     0.894212     319.00
 H       2.689623     4.710086     1.109025      30.49
 C       0.442069     3.374042    -0.632541      96.05
 H       0.272607     3.199021    -1.685549      23.79
 C      -0.321105     4.575138    -0.240764     102.01
 O       0.002571     5.833629    -0.787136     292.56
 H       0.115147     5.863096    -1.822421      26.25
 H      -0.174027     4.529704     0.895292      23.68
 H      -1.431849     4.522038    -0.481490      22.71
 C      -0.816486    -1.080997    -0.140645      75.24
 H      -0.611698    -2.136185     0.383579      21.92
 C      -2.879537     0.203661    -0.645882       2.84
 H      -3.915868     0.200283    -1.107412      21.97
 C      -2.287641     1.457503    -0.232729       8.79
 O      -2.933607     2.644916    -0.343567     202.73
 C      -4.351371     2.687019    -0.034199     107.10
 H      -4.959450     1.518100     0.328680      22.78
 H      -4.892806     3.668769     0.291102      24.88
 H      -4.725995     2.817315    -0.938376      28.06
 C      -0.840540     1.399308     0.091564     -29.16
 O       0.013239     2.455535     0.437560     138.95
 C      -0.060047     0.074664     0.160803      -0.13
 H       0.911119     0.240355     0.690779      22.24
 C      -2.065525    -1.096955    -0.628583       5.85
 C      -2.983131    -2.277652    -1.164892      76.61
 H      -3.949618    -2.059238    -1.439317      25.32
 O      -2.246369    -3.242844    -2.133827     172.48
 H      -2.765611    -4.105604    -1.952598      21.11
 C      -3.322065    -3.322473     0.198970      70.10
 H      -2.318648    -3.489414     0.536629      26.41
 O      -4.257126    -2.361548     0.974014     278.91
 H      -4.171988    -2.738892     1.782531      29.62
 C      -4.060430    -4.749064    -0.157796     107.02
 O      -3.252234    -5.570809    -1.084836     318.55
 H      -2.939565    -6.324065    -0.506514      26.04
 H      -5.095288    -4.679086    -0.559569      27.08
 H      -4.361992    -5.475005     0.560470      27.78
55
name = lig-etoh-frame_981
 C       2.520173     1.432837    -2.227238      59.49
 H       2.186873     1.996484    -3.132557      24.46
 C       3.523138     1.116479     0.052599      68.04
 H       3.930157     1.440167     0.973567      24.27
 C       4.297375     0.032111    -0.407824      12.38
 O       5.005266    -0.812041     0.447520     235.31
 C       4.981630    -0.513073     1.908179     103.65
 H       4.028148    -0.864811     2.325378      28.17
 H       4.929370     0.520041     2.181946      25.16
 H       5.828531    -1.117813     2.497482      24.54
 C       4.207901    -0.234047    -1.789546      21.20
 O       5.172322    -1.046877    -2.366336     259.19
 H       5.098981    -1.844056    -1.946062      31.33
 C       3.416304     0.429916    -2.700544      42.65
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 H       3.651650     0.317708    -3.709156      23.31
 C       2.739887     2.035597    -0.900576      25.98
 C       1.988424     3.435253    -0.425194      81.39
 H       2.391802     4.123852    -1.385365      21.52
 O       2.342343     3.916677     0.906967     260.75
 H       2.956288     4.757858     1.004293      25.24
 C       0.439726     3.427425    -0.635416      73.81
 H       0.174614     2.962701    -1.642902      22.29
 C      -0.317394     4.598721    -0.228890     115.54
 O       0.012634     5.830780    -0.779889     287.68
 H       0.226230     5.698642    -1.872786      23.17
 H      -0.269035     4.773109     0.816617      24.89
 H      -1.324575     4.222867    -0.408094      23.53
 C      -0.824052    -1.101423    -0.132668      55.11
 H      -0.439712    -2.042364     0.073831      22.03
 C      -2.802075     0.167441    -0.639471      52.65
 H      -3.674152     0.357383    -1.309995      20.89
 C      -2.268054     1.347340    -0.253437      -1.01
 O      -2.950997     2.647851    -0.264626     168.03
 C      -4.367041     2.679525    -0.076100      98.57
 H      -4.680967     1.836573     0.375596      26.48
 H      -4.308287     3.731347     0.519712      22.41
 H      -4.751748     2.770885    -1.333244      21.37
 C      -0.825081     1.369110     0.143498      -5.48
 O       0.029553     2.481566     0.483256     110.84
 C      -0.188310     0.095582     0.131405      32.22
 H       0.681502     0.040080     0.777734      23.32
 C      -2.115277    -1.074200    -0.684400      24.55
 C      -2.940278    -2.323682    -1.161330      69.43
 H      -4.042767    -2.066321    -1.430384      23.23
 O      -2.270376    -3.172097    -2.137459     235.86
 H      -2.606058    -3.995703    -1.851217      23.37
 C      -3.324336    -3.377878     0.199108      56.31
 H      -2.334232    -3.636040     0.760974      22.10
 O      -4.251749    -2.373853     0.980031     234.56
 H      -3.916060    -2.737933     2.031673      22.30
 C      -4.097263    -4.799662    -0.201999      78.42
 O      -3.273646    -5.588984    -1.054208     282.73
 H      -2.719789    -6.476112    -0.562699      22.61
 H      -5.069256    -4.403821    -0.754905      24.90
 H      -4.268923    -5.472576     0.733923      26.46
55
name = lig-etoh-frame_982
 C       2.502266     1.530349    -2.147705      77.81
 H       2.303501     2.218236    -2.974971      24.95
 C       3.509041     1.133342    -0.000198      57.60
 H       3.870831     1.599922     1.070318      20.70
 C       4.274687    -0.004756    -0.368324      11.59
 O       5.017627    -0.796475     0.449619     232.21
 C       4.923427    -0.506702     1.876507     109.45
 H       3.910303    -0.737811     2.297774      26.95
 H       5.001469     0.612780     1.921440      22.86
 H       5.869364    -1.002891     2.345689      25.18
 C       4.233396    -0.285265    -1.853078      10.18
 O       5.201533    -1.052527    -2.402722     145.18
 H       5.449177    -1.932576    -1.722607      22.22
 C       3.347826     0.435149    -2.711556      41.43
 H       3.635159     0.247679    -3.855239      23.72
 C       2.754644     2.060553    -0.888822      32.81
 C       2.061726     3.466365    -0.430906      93.67
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 H       2.075902     4.371724    -1.055908      21.84
 O       2.346315     3.932188     0.918141     273.17
 H       3.089280     4.548354     0.594741      25.91
 C       0.495085     3.405818    -0.610315      63.01
 H       0.126224     2.827914    -1.451943      23.73
 C      -0.364665     4.643735    -0.196733      97.86
 O       0.032739     5.849595    -0.803272     287.98
 H       0.247353     5.764226    -1.754732      27.67
 H      -0.288524     4.952185     0.911642      22.68
 H      -1.374635     4.134423    -0.370846      22.47
 C      -0.855730    -1.144634    -0.141647      11.57
 H      -0.013012    -2.049208    -0.281071      18.88
 C      -2.758433     0.125524    -0.691412      68.78
 H      -3.604125     0.290589    -1.325882      20.39
 C      -2.172689     1.330902    -0.241095       6.97
 O      -2.908712     2.602782    -0.184303     142.67
 C      -4.369715     2.745104    -0.194470     112.00
 H      -4.691227     1.834697     0.759907      22.38
 H      -4.156529     3.441856     0.614555      22.25
 H      -4.914777     2.727689    -0.979233      27.31
 C      -0.826636     1.341976     0.171977      34.18
 O       0.008228     2.473115     0.524657     120.36
 C      -0.305847     0.128185     0.156707      39.49
 H       0.644340    -0.088483     0.659600      23.34
 C      -2.212786    -1.079850    -0.749745      12.54
 C      -2.907696    -2.413038    -1.086315      89.89
 H      -3.803054    -1.998343    -1.506474      25.05
 O      -2.297053    -3.082288    -2.141286     216.15
 H      -2.295919    -4.140799    -1.931891      19.67
 C      -3.343482    -3.379421     0.182053      83.22
 H      -2.615091    -3.683958     0.948221      21.77
 O      -4.205667    -2.458444     1.000523     350.40
 H      -3.863620    -2.257860     1.923076      28.90
 C      -4.120581    -4.802855    -0.213552      94.35
 O      -3.277194    -5.627588    -1.046954     374.87
 H      -2.802245    -6.151036    -0.527486      31.95
 H      -4.901084    -4.431426    -0.821087      27.08
 H      -4.312741    -5.116366     0.774881      29.32
55
name = lig-etoh-frame_983
 C       2.554458     1.628590    -2.142575      43.92
 H       2.066494     2.419066    -2.753619      22.04
 C       3.509564     1.209658    -0.014552      58.28
 H       3.529231     1.633132     0.897620      23.16
 C       4.195743    -0.007840    -0.402100      16.44
 O       5.032394    -0.793456     0.447100     227.18
 C       4.872127    -0.460499     1.826608     126.36
 H       3.923215    -0.804975     2.227957      27.91
 H       5.197511     0.569573     1.876594      26.01
 H       5.772939    -0.964642     2.275727      26.88
 C       4.241620    -0.312927    -1.870765      10.19
 O       5.244011    -1.110561    -2.433656     202.34
 H       5.763923    -1.560340    -1.762070      26.35
 C       3.306927     0.452138    -2.684238      53.13
 H       3.305331     0.300805    -3.697810      26.99
 C       2.766676     2.061348    -0.841970      37.01
 C       2.085123     3.467325    -0.460354      98.05
 H       2.216126     4.544421    -0.941635      19.62
 O       2.374421     3.945944     0.908478     292.04
 H       3.161974     4.357458     0.667132      29.86
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 C       0.539155     3.334132    -0.508151      57.60
 H       0.214595     2.918891    -1.493833      21.06
 C      -0.406070     4.669115    -0.155580      92.10
 O       0.040454     5.887076    -0.810521     246.65
 H       0.234417     5.861757    -1.962089      19.27
 H      -0.272629     4.821181     0.884534      23.95
 H      -1.446038     4.494351    -0.390995      23.39
 C      -0.896619    -1.179604    -0.207000      63.99
 H      -0.158811    -1.787605    -0.429255      24.08
 C      -2.773722     0.154232    -0.779166      32.07
 H      -3.862070     0.200141    -1.212537      24.71
 C      -2.116042     1.375709    -0.231654      20.20
 O      -2.821761     2.523089    -0.138406     157.46
 C      -4.320036     2.746576    -0.153883     102.56
 H      -4.793065     2.056441     0.457200      27.36
 H      -4.617142     3.702715     0.479902      24.81
 H      -5.336166     2.764862    -1.046703      22.26
 C      -0.840198     1.391977     0.192093      26.93
 O      -0.034792     2.437382     0.570111     207.14
 C      -0.331997     0.038912     0.227424      18.12
 H       0.784046     0.066141     0.408473      24.77
 C      -2.198557    -1.190148    -0.749945       3.57
 C      -2.920272    -2.482597    -0.983111     105.30
 H      -3.869148    -2.081726    -1.500136      22.84
 O      -2.294120    -3.037810    -2.167037     243.23
 H      -1.999091    -3.957931    -2.080321      23.32
 C      -3.374997    -3.346765     0.183025      95.57
 H      -2.571910    -3.698521     0.880367      21.38
 O      -4.177772    -2.542835     0.979371     376.40
 H      -3.743164    -2.239927     1.793655      31.55
 C      -4.100062    -4.717481    -0.220617      69.16
 O      -3.293812    -5.649730    -1.052878     299.85
 H      -2.658752    -6.141294    -0.194560      21.82
 H      -5.094243    -4.605524    -0.948034      23.62
 H      -4.559264    -5.014506     0.809536      25.65
55
name = lig-etoh-frame_984
 C       2.645722     1.704124    -2.184115      32.16
 H       1.817632     2.251856    -2.693365      21.15
 C       3.524419     1.270341    -0.010425      59.83
 H       3.320411     1.573304     1.175703      20.52
 C       4.120622     0.010719    -0.476711      10.32
 O       5.020952    -0.784302     0.406526     212.25
 C       4.871886    -0.406453     1.773877     106.26
 H       3.897458    -0.785007     2.193827      27.46
 H       5.131928     0.636830     2.056768      25.39
 H       5.626427    -1.156716     2.405002      25.52
 C       4.228902    -0.299745    -1.848210       7.47
 O       5.263019    -1.163061    -2.465082     176.00
 H       5.951038    -1.306522    -1.729037      24.14
 C       3.278312     0.501054    -2.617036      47.92
 H       2.968352     0.297938    -3.749969      24.70
 C       2.763427     2.081318    -0.823889      41.91
 C       2.068847     3.470983    -0.451833     101.04
 H       2.476900     4.186840    -1.203882      24.44
 O       2.414873     3.945471     0.899851     254.38
 H       3.401338     4.307442     1.071726      26.39
 C       0.511464     3.283146    -0.404616      73.14
 H       0.347179     3.061099    -1.476466      21.57
 C      -0.394093     4.683910    -0.155747      87.17
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 O       0.044669     5.929823    -0.813968     252.37
 H       0.202173     5.781188    -1.813129      24.84
 H      -0.259205     4.750602     0.980683      23.01
 H      -1.488343     4.698803    -0.444847      22.30
 C      -0.916912    -1.158667    -0.270824      50.86
 H      -0.150072    -2.116566    -0.511340      22.24
 C      -2.806881     0.164819    -0.856378      37.84
 H      -3.845424     0.229820    -0.938523      27.09
 C      -2.172284     1.365951    -0.272731       6.03
 O      -2.786571     2.509915    -0.109411     157.61
 C      -4.311582     2.771943    -0.088424     107.96
 H      -5.001748     1.780291     0.400400      23.45
 H      -4.718791     3.774091    -0.002653      25.38
 H      -4.756973     2.754645    -1.007109      27.23
 C      -0.808481     1.359957     0.215097       6.19
 O      -0.064780     2.407899     0.615160     195.28
 C      -0.288203    -0.029484     0.289010      35.41
 H       0.771135     0.098223     0.230638      25.57
 C      -2.182629    -1.240400    -0.698484       9.57
 C      -2.977578    -2.500377    -0.956746      93.96
 H      -4.005705    -2.325012    -1.273662      24.03
 O      -2.265752    -3.015112    -2.210989     222.74
 H      -1.861727    -3.857144    -2.053061      23.83
 C      -3.368552    -3.361772     0.189990     103.65
 H      -2.354979    -3.709656     0.586277      22.47
 O      -4.201785    -2.599021     0.938610     326.88
 H      -3.538776    -2.504073     1.869351      22.38
 C      -4.126392    -4.613532    -0.252471     103.58
 O      -3.298670    -5.665474    -0.994755     357.78
 H      -2.731503    -6.187401    -0.412525      30.31
 H      -4.975371    -4.571538    -0.813028      27.13
 H      -4.588422    -5.123655     0.566617      26.54
55
name = lig-etoh-frame_985
 C       2.719526     1.749171    -2.208822      53.29
 H       1.840801     1.919611    -2.851849      22.66
 C       3.519613     1.299826     0.048832      67.14
 H       3.456085     1.303775     1.031393      24.90
 C       4.101991     0.043116    -0.503966      15.62
 O       4.981231    -0.745853     0.338630     216.74
 C       4.889014    -0.403719     1.768926     112.03
 H       3.851651    -0.580011     2.079844      29.20
 H       4.986276     0.629740     2.108498      26.71
 H       5.480452    -1.110942     2.314520      28.53
 C       4.212176    -0.262060    -1.854893       4.25
 O       5.231088    -1.197809    -2.469781     152.31
 H       6.045772    -1.032132    -1.730289      22.96
 C       3.258146     0.554655    -2.607087      45.69
 H       2.957897     0.201185    -3.535840      26.24
 C       2.754371     2.124070    -0.829730      32.43
 C       2.074225     3.453562    -0.388822      90.87
 H       2.441118     3.784104    -1.449266      20.99
 O       2.463853     3.949744     0.899995     292.76
 H       3.382954     4.075099     1.262852      28.27
 C       0.448582     3.316506    -0.352619      70.24
 H       0.236945     2.919823    -1.355414      22.93
 C      -0.351289     4.703342    -0.154629     104.43
 O       0.045370     5.956220    -0.767096     262.91
 H       0.269162     5.686938    -1.834957      22.63
 H      -0.336223     4.892768     0.904909      24.31
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 H      -1.369574     4.461242    -0.428155      23.38
 C      -0.837553    -1.188105    -0.318101      42.95
 H      -0.492309    -2.134510    -0.298846      25.28
 C      -2.808670     0.136626    -0.872677      57.41
 H      -3.972668     0.249537    -0.792204      24.74
 C      -2.229432     1.284191    -0.327338      -8.84
 O      -2.816601     2.580795    -0.069390     136.29
 C      -4.319332     2.729523    -0.060237     107.01
 H      -4.783451     2.009435     0.438932      27.65
 H      -4.420735     3.854815     0.056359      24.51
 H      -4.075265     2.497064    -1.384265      18.41
 C      -0.808508     1.199484     0.213711       3.71
 O      -0.072247     2.395282     0.653995     143.87
 C      -0.223044    -0.017387     0.297506      53.98
 H       0.923809    -0.137775     0.301779      23.99
 C      -2.257915    -1.178661    -0.651181     -11.82
 C      -3.032305    -2.477135    -1.023104      72.79
 H      -4.077766    -2.284366    -1.303908      24.53
 O      -2.246185    -3.001098    -2.247704     170.47
 H      -1.799095    -3.901285    -1.876143      19.83
 C      -3.294564    -3.449522     0.153537     102.06
 H      -2.348451    -3.732674     0.587309      23.60
 O      -4.217938    -2.625029     0.960527     318.59
 H      -3.981793    -2.741295     1.838139      29.81
 C      -4.125923    -4.594064    -0.281348      72.33
 O      -3.325243    -5.644499    -0.953284     306.90
 H      -2.722947    -6.351187    -0.313656      23.50
 H      -5.057095    -4.197094    -1.057525      23.05
 H      -4.504190    -5.203912     0.590921      24.82
55
name = lig-etoh-frame_986
 C       2.738931     1.766861    -2.212117      59.27
 H       1.973460     1.967548    -2.983817      22.60
 C       3.495795     1.276817     0.038692      62.28
 H       3.589022     1.287694     1.236401      20.95
 C       4.143127     0.096969    -0.477892      18.62
 O       4.933336    -0.683373     0.279480     205.30
 C       4.858718    -0.408475     1.753948      92.26
 H       3.777387    -0.514114     1.987616      27.83
 H       5.150812     0.629508     1.955833      25.54
 H       5.635618    -1.249128     2.319529      24.91
 C       4.196378    -0.212561    -1.897575      11.36
 O       5.162271    -1.185562    -2.433082     238.11
 H       5.884134    -1.057793    -1.943644      30.00
 C       3.299406     0.553900    -2.624144      59.04
 H       3.040610     0.078860    -3.643428      25.08
 C       2.762696     2.144981    -0.799988      45.71
 C       2.079092     3.387881    -0.343184      95.10
 H       2.152648     4.095896    -1.224154      24.48
 O       2.493739     3.960247     0.909627     311.85
 H       3.415222     3.815624     1.042818      30.35
 C       0.410968     3.380230    -0.342106      56.64
 H       0.047717     2.787771    -1.219846      22.75
 C      -0.312956     4.710258    -0.135790     108.71
 O       0.052700     5.943466    -0.727048     269.55
 H       0.251758     5.940074    -1.661849      28.82
 H      -0.402817     5.037221     0.940800      23.46
 H      -1.300649     4.221136    -0.436531      22.22
 C      -0.828985    -1.205452    -0.332196      24.80
 H      -0.484690    -2.334653    -0.027030      22.74
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 C      -2.874951     0.110808    -0.828200      69.85
 H      -3.906874     0.123139    -0.949858      27.05
 C      -2.220704     1.247045    -0.331247      -7.69
 O      -2.818701     2.626873    -0.001486     108.62
 C      -4.234933     2.699451    -0.190694     110.14
 H      -4.844191     2.018740     0.781647      23.22
 H      -4.280606     3.708375     0.267473      24.20
 H      -4.359632     2.402463    -1.084156      27.27
 C      -0.856288     1.100494     0.187091      -3.16
 O      -0.089478     2.367866     0.685905      61.71
 C      -0.110934    -0.068658     0.237197      42.59
 H       0.857416    -0.219794     0.622536      24.39
 C      -2.299136    -1.096621    -0.625872     -19.06
 C      -3.049507    -2.425902    -1.116656      63.90
 H      -4.034552    -2.081495    -1.564515      22.99
 O      -2.237204    -3.005897    -2.252866     215.51
 H      -1.921500    -3.810117    -1.850029      23.23
 C      -3.227709    -3.498666     0.104058      80.74
 H      -2.364257    -3.785141     0.830290      20.41
 O      -4.226080    -2.647389     0.979247     193.64
 H      -4.361435    -2.949970     2.046406      24.37
 C      -4.135210    -4.650506    -0.322396      95.41
 O      -3.341998    -5.621106    -0.940043     327.75
 H      -2.995318    -6.257813    -0.173270      26.38
 H      -4.717145    -4.150877    -0.942073      29.22
 H      -4.615040    -4.963599     0.621634      28.51
55
name = lig-etoh-frame_987
 C       2.715763     1.754291    -2.197701      62.84
 H       2.134042     2.419390    -2.895649      20.89
 C       3.468705     1.222267     0.041392      70.33
 H       3.590353     1.611058     1.034360      23.01
 C       4.195857     0.179173    -0.487872      28.62
 O       4.909813    -0.638734     0.264831     217.08
 C       4.844756    -0.437109     1.718787     117.29
 H       3.819632    -0.578016     2.074983      27.64
 H       5.410976     0.510224     1.828508      25.65
 H       5.454775    -1.115897     2.125606      29.33
 C       4.213572    -0.169377    -1.894011      22.46
 O       5.035838    -1.148464    -2.399083     162.14
 H       5.970639    -1.161062    -1.893536      24.82
 C       3.359621     0.525482    -2.697130      57.67
 H       3.238592     0.241111    -3.754010      27.23
 C       2.779355     2.138362    -0.800503      55.20
 C       2.021945     3.364476    -0.331081     102.78
 H       2.014229     4.434497    -0.769430      20.23
 O       2.521437     3.965038     0.927937     280.95
 H       3.489442     3.584493     0.739055      26.57
 C       0.427751     3.370543    -0.331242      57.47
 H       0.051674     2.991318    -1.279748      23.09
 C      -0.322203     4.696682    -0.091522     107.77
 O       0.065099     5.922545    -0.679633     228.91
 H       0.181513     6.080384    -1.779958      22.53
 H      -0.406806     4.942852     0.978742      24.62
 H      -1.329891     4.454524    -0.430530      24.32
 C      -0.872018    -1.242276    -0.289206      39.93
 H      -0.458459    -2.142229     0.028095      24.13
 C      -2.972277     0.130968    -0.749141      42.21
 H      -4.029611     0.065549    -1.234688      22.60
 C      -2.175507     1.279951    -0.279463      10.33
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 O      -2.768674     2.599794     0.051607     142.69
 C      -4.152966     2.665573    -0.208309     106.51
 H      -4.654746     2.176246     0.484084      28.82
 H      -4.506526     3.678183     0.100672      26.08
 H      -5.117814     2.336473    -1.306065      21.75
 C      -0.876839     1.110753     0.157881     -15.20
 O      -0.132213     2.320925     0.710008      80.96
 C      -0.050497    -0.174981     0.131841      -3.36
 H       0.809670    -0.106648     0.916906      20.58
 C      -2.252458    -1.101112    -0.639931       8.08
 C      -3.010208    -2.358847    -1.180959      74.92
 H      -3.895847    -2.063648    -1.676822      26.02
 O      -2.242418    -3.007816    -2.241388     233.60
 H      -1.982435    -3.870372    -1.906076      24.52
 C      -3.224299    -3.471089     0.101112      91.46
 H      -2.413970    -3.721161     0.725324      24.39
 O      -4.230814    -2.670159     0.982546     214.02
 H      -4.323843    -3.135067     1.884592      25.93
 C      -4.108299    -4.690509    -0.312062      70.36
 O      -3.361172    -5.627234    -0.946464     333.95
 H      -3.041278    -6.200114    -0.267556      29.95
 H      -4.868694    -4.150099    -1.197410      23.69
 H      -4.845953    -4.834330     0.523120      28.00
55
name = lig-etoh-frame_988
 C       2.682057     1.731646    -2.185103      68.87
 H       2.406419     2.660086    -2.694479      23.54
 C       3.424961     1.232609     0.040923      71.52
 H       3.602956     1.727821     1.035267      23.23
 C       4.239864     0.259612    -0.528620      30.63
 O       4.917009    -0.638384     0.282712     240.42
 C       4.849013    -0.439197     1.648377      97.12
 H       3.882161    -0.495621     2.210230      26.39
 H       5.405573     0.456447     1.958041      25.15
 H       5.524686    -1.480827     2.103118      22.92
 C       4.238870    -0.115932    -1.855683      25.65
 O       4.920809    -1.117070    -2.368696     184.71
 H       5.797963    -1.418284    -1.815696      23.38
 C       3.391217     0.570921    -2.786829      45.96
 H       3.438675     0.442543    -3.875242      23.79
 C       2.777205     2.112164    -0.867380      41.91
 C       1.909897     3.422845    -0.313989     103.32
 H       2.158572     4.312559    -0.905730      23.36
 O       2.570813     3.927416     0.959224     280.45
 H       3.520629     3.704053     0.803026      29.05
 C       0.451444     3.299740    -0.314394      61.92
 H       0.220091     3.176075    -1.419605      21.96
 C      -0.371275     4.677431    -0.035424      96.99
 O       0.097443     5.918352    -0.655174     237.68
 H       0.033438     5.729601    -1.568458      29.73
 H      -0.335900     4.790095     1.064287      24.69
 H      -1.437693     4.681903    -0.375775      23.90
 C      -0.905875    -1.265572    -0.209489      40.78
 H      -0.460783    -2.345046    -0.064343      20.32
 C      -3.018299     0.152571    -0.654032      33.17
 H      -3.866383     0.222278    -1.315624      19.52
 C      -2.186356     1.322646    -0.214003       7.50
 O      -2.704711     2.534237     0.055638     154.87
 C      -4.163870     2.667127    -0.246093     107.95
 H      -4.714093     1.805305     0.588346      23.48
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 H      -4.576693     3.701241    -0.296871      25.43
 H      -4.830830     2.473446    -1.001722      26.35
 C      -0.791581     1.145516     0.138383      -5.28
 O      -0.191875     2.264363     0.701207     127.81
 C      -0.089707    -0.193065     0.046023      27.79
 H       0.672095    -0.101200     0.763057      23.22
 C      -2.220458    -1.122638    -0.700867      17.93
 C      -2.925367    -2.323685    -1.180261      79.82
 H      -3.968517    -2.086849    -1.637719      24.82
 O      -2.237277    -3.010088    -2.234350     203.33
 H      -2.067162    -4.041716    -1.986897      20.02
 C      -3.321862    -3.372335     0.102067      76.20
 H      -2.233439    -3.627260     0.530224      22.31
 O      -4.220514    -2.698398     0.946077     264.36
 H      -4.088812    -3.130546     1.791154      26.49
 C      -4.129593    -4.621064    -0.335175      95.28
 O      -3.380674    -5.668120    -0.976480     298.25
 H      -2.728989    -6.441463    -0.342996      21.82
 H      -4.767227    -4.451402    -1.075078      26.92
 H      -4.903646    -5.023878     0.376817      27.57
55
name = lig-etoh-frame_989
 C       2.674669     1.717511    -2.227012      74.56
 H       2.447507     2.585508    -2.863076      24.16
 C       3.389362     1.309997     0.031317      67.28
 H       3.602675     1.542711     1.153129      22.13
 C       4.271423     0.317807    -0.512085      28.77
 O       4.932394    -0.653099     0.278546     248.81
 C       4.910505    -0.492576     1.652583     126.39
 H       3.898907    -0.402193     2.097629      27.76
 H       5.357790     0.406037     2.109565      26.47
 H       5.307692    -1.322184     1.952145      29.05
 C       4.212042    -0.022168    -1.875968      27.16
 O       4.852864    -1.139975    -2.350607     227.34
 H       5.367940    -1.541695    -1.754652      28.74
 C       3.412529     0.689025    -2.821569      53.27
 H       3.645426     0.606452    -3.951598      22.27
 C       2.724010     2.089729    -0.889360      32.35
 C       1.903423     3.482528    -0.292935      88.85
 H       2.174972     4.029483    -1.298844      22.64
 O       2.602550     3.869467     0.992679     283.19
 H       3.540316     3.913929     0.931419      29.88
 C       0.405480     3.255902    -0.307526      64.90
 H       0.320445     3.005812    -1.369119      22.37
 C      -0.425155     4.661060     0.042518      94.80
 O       0.134939     5.879169    -0.616643     214.85
 H       0.019171     5.535800    -1.591002      25.97
 H      -0.266441     4.742513     1.152766      24.22
 H      -1.493543     4.560732    -0.233750      23.96
 C      -0.931775    -1.322650    -0.140574      34.20
 H      -0.589234    -2.359041    -0.311414      20.37
 C      -2.940051     0.159228    -0.564527      60.52
 H      -3.815613     0.394272    -1.215525      20.30
 C      -2.203743     1.282249    -0.158661       2.75
 O      -2.683913     2.501952     0.024096     135.48
 C      -4.208270     2.652284    -0.189668      85.97
 H      -4.603232     2.046188     0.446877      28.40
 H      -4.321998     3.751769    -0.211711      24.81
 H      -4.259270     2.103286    -1.551096      19.94
 C      -0.720564     1.140907     0.096318      23.52
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 O      -0.220764     2.235031     0.653041     176.93
 C      -0.189211    -0.104128     0.008046      43.27
 H       0.876711    -0.272867     0.470464      21.62
 C      -2.229406    -1.093770    -0.755451       7.29
 C      -2.912567    -2.340712    -1.154176      94.08
 H      -3.862650    -2.052278    -1.476170      27.39
 O      -2.209063    -3.037596    -2.235477     245.54
 H      -2.300230    -3.950675    -2.035617      24.45
 C      -3.394515    -3.272934     0.056533      95.44
 H      -2.442583    -3.537611     0.372844      25.30
 O      -4.216401    -2.708875     0.910753     315.39
 H      -3.800039    -2.851163     1.992272      21.39
 C      -4.139245    -4.583530    -0.359714      77.48
 O      -3.364096    -5.744680    -1.009798     358.65
 H      -2.787358    -6.206576    -0.489094      32.37
 H      -4.938878    -4.406216    -1.317325      22.44
 H      -4.666118    -5.123637     0.445743      25.39
55
name = lig-etoh-frame_990
 C       2.669956     1.767094    -2.310823      74.69
 H       2.175259     2.331029    -3.133418      22.83
 C       3.416924     1.363904     0.037234      64.14
 H       3.409658     1.467575     1.063521      21.16
 C       4.267640     0.355389    -0.473067      31.90
 O       4.952639    -0.651543     0.235396     229.56
 C       4.941903    -0.512522     1.700169      93.57
 H       3.840742    -0.454358     1.878007      25.80
 H       5.531807     0.354410     2.082890      24.99
 H       5.386438    -1.671972     2.164807      22.74
 C       4.179736     0.052800    -1.922170      28.99
 O       4.797164    -1.167536    -2.355888     124.32
 H       5.041032    -1.747539    -1.420688      21.44
 C       3.469947     0.812936    -2.827565      41.77
 H       3.651412     0.712360    -3.830030      22.90
 C       2.615207     2.099478    -0.854066      47.44
 C       2.003748     3.475522    -0.300139      94.51
 H       2.029597     4.015231    -1.230987      22.80
 O       2.587881     3.808838     1.004634     253.34
 H       3.585876     4.189552     0.876152      26.09
 C       0.330043     3.269618    -0.287549      59.89
 H       0.149332     2.727902    -1.265668      20.99
 C      -0.443397     4.627841     0.123714     103.20
 O       0.150692     5.785441    -0.572662     229.05
 H       0.225471     5.771491    -1.640580      23.82
 H      -0.288497     4.808859     1.174871      25.10
 H      -1.491093     4.369642    -0.062747      23.95
 C      -0.995460    -1.325788    -0.149876      22.80
 H      -0.503986    -2.298023    -0.373697      20.16
 C      -2.834063     0.144546    -0.528471      72.90
 H      -3.889745     0.363963    -0.872039      20.77
 C      -2.157104     1.196901    -0.102316      17.29
 O      -2.709359     2.506155    -0.004504     150.88
 C      -4.150571     2.632079    -0.240623      91.48
 H      -4.936073     2.028976     0.676393      22.64
 H      -4.194506     3.739237    -0.006329      23.86
 H      -4.001811     2.136204    -1.365814      20.62
 C      -0.774881     1.130786     0.039256      24.70
 O      -0.187773     2.259284     0.594615     188.46
 C      -0.211959    -0.085810     0.035566      31.94
 H       0.852116    -0.257294    -0.139711      22.79
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 C      -2.221443    -1.072691    -0.741166      18.41
 C      -2.974102    -2.355777    -1.147603      77.79
 H      -3.966235    -1.929281    -1.628467      24.63
 O      -2.181207    -3.065767    -2.225216     186.80
 H      -2.515328    -4.033273    -2.088315      20.98
 C      -3.395259    -3.250126    -0.055236      79.20
 H      -2.440606    -3.656506     0.571527      20.43
 O      -4.233968    -2.667319     0.960963     375.62
 H      -3.887962    -2.472758     1.753582      34.00
 C      -4.155068    -4.608318    -0.453919      82.75
 O      -3.369327    -5.770945    -1.079202     279.40
 H      -2.654693    -6.123113    -0.196099      21.10
 H      -4.883590    -4.298271    -1.049905      27.80
 H      -4.417638    -4.937218     0.603866      26.19
55
name = lig-etoh-frame_991
 C       2.623001     1.895398    -2.353438      66.99
 H       1.820427     2.152912    -3.077588      20.38
 C       3.464826     1.389696     0.022590      58.46
 H       3.159077     1.603810     1.177737      19.62
 C       4.237471     0.359725    -0.489264      13.94
 O       4.985720    -0.636488     0.194740     227.49
 C       4.965704    -0.587520     1.746573     119.74
 H       3.900519    -0.486534     1.949331      27.40
 H       5.637379     0.214372     1.991295      27.08
 H       5.284900    -1.391691     2.116566      30.37
 C       4.199806     0.062300    -1.911856      10.48
 O       4.754716    -1.185498    -2.332571     184.57
 H       4.617973    -1.680669    -1.477880      24.43
 C       3.555717     0.911847    -2.821073      35.89
 H       3.562698     0.691837    -3.999511      21.52
 C       2.516708     2.127412    -0.852807      71.72
 C       2.058081     3.395528    -0.321841     111.84
 H       2.118127     4.413710    -0.964711      22.60
 O       2.569578     3.763239     0.989064     275.03
 H       3.299771     4.356910     0.792736      29.97
 C       0.290179     3.306648    -0.267865      73.80
 H      -0.050981     2.946232    -1.255061      23.50
 C      -0.421640     4.570138     0.155012     104.05
 O       0.155264     5.698156    -0.529992     262.83
 H       0.263082     5.736173    -1.454564      29.60
 H      -0.264300     4.887388     1.251451      24.38
 H      -1.544346     4.380313     0.034750      24.10
 C      -1.002673    -1.268066    -0.207243      38.99
 H      -0.327664    -2.199665    -0.295444      22.33
 C      -2.819802     0.103755    -0.539881      60.91
 H      -3.884932     0.115108    -0.518483      24.76
 C      -2.124514     1.207519    -0.044940      27.31
 O      -2.728042     2.489740    -0.002069     206.59
 C      -4.069488     2.605680    -0.226772     126.70
 H      -4.778720     2.200730     0.286249      30.09
 H      -4.332109     3.620623    -0.111570      27.55
 H      -4.466241     2.339046    -1.486272      24.10
 C      -0.826334     1.156470     0.030355      -0.60
 O      -0.127710     2.283358     0.560212     188.61
 C      -0.182432    -0.174059     0.046142      29.19
 H       0.841745    -0.108576    -0.401811      22.88
 C      -2.238875    -1.137204    -0.685906      42.05
 C      -3.066372    -2.310951    -1.207826      91.72
 H      -3.868482    -1.998542    -1.789014      25.37
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 O      -2.171867    -3.101687    -2.185979     186.21
 H      -2.614825    -4.041409    -2.280210      21.97
 C      -3.342421    -3.308025    -0.089260      89.07
 H      -2.568668    -3.633448     0.482060      22.85
 O      -4.289051    -2.608104     0.964602     268.62
 H      -3.726880    -2.211641     1.856682      24.31
 C      -4.117760    -4.649663    -0.504697      80.58
 O      -3.371355    -5.751645    -1.120264     350.25
 H      -2.881840    -6.116474    -0.452009      32.01
 H      -5.205524    -4.323470    -1.039443      24.64
 H      -4.410117    -4.791483     0.514864      26.36
55
name = lig-etoh-frame_992
 C       2.571845     1.997223    -2.334992      60.65
 H       1.642419     2.211003    -2.882121      20.98
 C       3.445364     1.431483     0.003224      40.14
 H       3.336748     1.671828     0.958098      21.77
 C       4.210224     0.329917    -0.519788       4.60
 O       5.017509    -0.619379     0.182786     206.47
 C       4.961198    -0.616299     1.715865      86.51
 H       3.981770    -0.399838     2.232702      26.57
 H       5.660066     0.232689     2.025861      24.72
 H       5.442852    -1.775187     2.147251      23.27
 C       4.240569     0.059620    -1.896624       7.88
 O       4.706508    -1.175057    -2.297588     216.06
 H       4.513582    -1.753968    -1.563731      27.31
 C       3.606258     1.005168    -2.836698      32.52
 H       3.498830     0.671226    -3.791412      22.62
 C       2.518232     2.123719    -0.920026      52.17
 C       2.000071     3.389923    -0.344937     115.47
 H       2.323992     4.331567    -0.663979      23.71
 O       2.539779     3.715116     0.972177     265.75
 H       3.099920     4.471925     0.831757      29.56
 C       0.303827     3.350785    -0.286532      69.66
 H      -0.072283     3.412991    -1.378110      22.49
 C      -0.396239     4.540408     0.191163     116.04
 O       0.155782     5.645888    -0.472033     225.55
 H       0.133578     5.406628    -1.570128      25.35
 H      -0.210279     4.743049     1.210742      25.93
 H      -1.456808     4.537935     0.033062      25.67
 C      -0.892937    -1.256028    -0.277097      53.82
 H      -0.404632    -2.176532    -0.280847      24.70
 C      -2.868721     0.067015    -0.544927      43.04
 H      -4.000413    -0.073666    -0.311228      23.15
 C      -2.198147     1.253796    -0.031392      12.42
 O      -2.721286     2.460438     0.023612     175.31
 C      -4.032520     2.636391    -0.253994      93.91
 H      -4.884330     1.796178     0.328019      22.63
 H      -4.417980     3.712040    -0.306179      23.68
 H      -4.751408     2.422999    -1.675514      21.26
 C      -0.742487     1.153602     0.087007      -7.23
 O      -0.069327     2.259904     0.560506     178.04
 C      -0.152699    -0.180205     0.024262      63.33
 H       0.938832    -0.101974    -0.230222      22.78
 C      -2.315186    -1.224739    -0.640569      13.94
 C      -3.096116    -2.298939    -1.271022      87.44
 H      -3.980658    -2.011056    -1.917257      21.53
 O      -2.174885    -3.131388    -2.146252     228.03
 H      -2.594112    -3.915073    -2.354322      25.97
 C      -3.358907    -3.354857    -0.093923      60.79
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 H      -2.276435    -3.609600     0.406431      19.98
 O      -4.330470    -2.548572     0.933699     265.74
 H      -3.690785    -2.410933     1.696058      26.17
 C      -4.114093    -4.650476    -0.525682     102.90
 O      -3.403223    -5.693319    -1.179107     281.18
 H      -2.826322    -6.358475    -0.451116      23.00
 H      -5.012009    -4.634096    -1.026510      25.63
 H      -4.554654    -5.031946     0.483666      24.52
55
name = lig-etoh-frame_993
 C       2.567151     2.004426    -2.304741      64.78
 H       1.739364     2.462744    -2.873925      23.26
 C       3.409436     1.438540    -0.086102      48.11
 H       3.637209     1.797890     1.062576      20.02
 C       4.186567     0.313912    -0.512865      16.99
 O       5.024714    -0.598911     0.208653     235.44
 C       4.992790    -0.660920     1.681468     130.18
 H       4.101720    -0.431324     2.261077      28.91
 H       5.628007     0.091878     2.059643      28.31
 H       5.320368    -1.539873     1.823215      30.53
 C       4.244184     0.102572    -1.916460      20.63
 O       4.671096    -1.149286    -2.281854     159.84
 H       4.585538    -1.973064    -1.534941      22.45
 C       3.596610     1.081226    -2.799705      55.39
 H       3.490900     0.632204    -3.888585      20.08
 C       2.594299     2.128839    -0.967995      36.54
 C       1.876046     3.432008    -0.331621      98.26
 H       2.344455     4.241694    -1.099458      21.41
 O       2.500738     3.646947     0.981818     258.88
 H       2.926310     4.620017     1.008361      26.64
 C       0.364345     3.384132    -0.349363      75.94
 H       0.060067     3.433855    -1.398640      22.64
 C      -0.373436     4.553343     0.267322     104.78
 O       0.163889     5.626924    -0.465089     250.26
 H       0.031993     5.343435    -1.334351      32.16
 H      -0.141081     4.566277     1.398403      23.72
 H      -1.507242     4.550375     0.031949      23.76
 C      -0.836526    -1.311994    -0.378857       8.71
 H      -0.392302    -2.417926    -0.383715      21.80
 C      -2.964466     0.041285    -0.498443      58.46
 H      -4.002259     0.020243    -0.445154      26.74
 C      -2.216331     1.201843    -0.063074      -7.66
 O      -2.721505     2.471079     0.049741     171.65
 C      -4.151836     2.641325    -0.339954     133.23
 H      -4.502441     1.948006     0.227084      29.85
 H      -4.281582     3.704588    -0.180125      27.33
 H      -4.307578     2.441660    -1.179345      33.48
 C      -0.700250     1.119186     0.157984      20.02
 O      -0.002694     2.216986     0.563532     137.54
 C      -0.092577    -0.082496    -0.007635      55.77
 H       0.995210    -0.252745     0.201058      22.87
 C      -2.323420    -1.243199    -0.602366     -27.46
 C      -3.092362    -2.377312    -1.304164      93.26
 H      -3.985073    -1.982231    -1.820505      21.08
 O      -2.168175    -3.128348    -2.116670     207.37
 H      -2.698542    -4.004268    -2.364158      19.47
 C      -3.421238    -3.359445    -0.087028      84.58
 H      -2.437120    -3.506114     0.181605      24.80
 O      -4.333190    -2.526410     0.861304     335.64
 H      -3.843744    -2.612638     1.702825      28.23
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 C      -4.127348    -4.678444    -0.462761      92.27
 O      -3.406081    -5.650033    -1.230403     303.28
 H      -2.906393    -6.382651    -0.667724      25.75
 H      -5.047725    -4.563114    -1.286224      21.74
 H      -4.531065    -5.236067     0.337271      25.03
55
name = lig-etoh-frame_994
 C       2.605056     1.953047    -2.321424      59.46
 H       2.112698     2.684454    -2.993675      25.78
 C       3.427378     1.402277    -0.113239      64.47
 H       3.732226     1.860619     0.768510      24.28
 C       4.172286     0.326284    -0.505403      22.62
 O       4.998724    -0.561338     0.237426     233.78
 C       5.022522    -0.652337     1.629857      93.43
 H       3.969229    -0.573481     2.066841      25.85
 H       5.836125     0.023670     2.128261      24.17
 H       5.409973    -1.905021     1.749603      22.74
 C       4.202887     0.159291    -1.915346      29.42
 O       4.658055    -1.139034    -2.301584     211.27
 H       4.733461    -1.678427    -1.538308      25.92
 C       3.547590     1.080338    -2.787089      71.43
 H       3.574196     0.861812    -3.822961      20.03
 C       2.640120     2.201277    -0.929950      44.94
 C       1.835676     3.488183    -0.346930      98.43
 H       2.002300     3.988719    -1.255046      22.93
 O       2.447937     3.599338     0.989780     315.69
 H       2.635439     4.519621     1.189560      29.94
 C       0.405189     3.386697    -0.381977      63.17
 H       0.106489     3.054588    -1.445020      21.24
 C      -0.363359     4.559265     0.357927     112.52
 O       0.177515     5.657574    -0.451041     222.38
 H       0.005326     5.482202    -1.444809      27.66
 H      -0.116177     4.563723     1.386547      25.93
 H      -1.388480     4.388771     0.235040      25.64
 C      -0.843035    -1.360026    -0.476053      18.79
 H      -0.367906    -2.256671    -0.541259      23.44
 C      -3.018403     0.023399    -0.417838      51.48
 H      -4.141114     0.201936    -0.729363      20.57
 C      -2.182872     1.117200    -0.108744      -6.21
 O      -2.720721     2.492542     0.063603      67.30
 C      -4.207012     2.678976    -0.355573      50.22
 H      -4.744229     1.902531     0.565496      21.32
 H      -4.339081     3.706721     0.079463      22.91
 H      -4.036414     2.196988    -1.846645      18.52
 C      -0.747367     1.096091     0.201608       4.43
 O       0.068414     2.182898     0.560732      84.10
 C      -0.022520    -0.079735    -0.047340     -23.52
 H       0.862020    -0.283841     0.634189      20.94
 C      -2.255313    -1.220452    -0.598860       4.15
 C      -3.075230    -2.468563    -1.268127      92.22
 H      -3.947487    -2.014780    -1.784805      26.09
 O      -2.168680    -3.130830    -2.116027     240.60
 H      -2.607621    -4.028261    -2.265912      21.97
 C      -3.537581    -3.325706    -0.093859      84.11
 H      -2.445199    -3.572090     0.369539      22.30
 O      -4.295918    -2.532005     0.768459     278.36
 H      -4.254219    -2.870518     1.862624      24.12
 C      -4.196665    -4.724297    -0.432563      92.57
 O      -3.382814    -5.618814    -1.296240     329.41
 H      -2.928697    -6.230709    -0.720337      28.49
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 H      -4.867036    -4.239282    -1.096048      26.35
 H      -4.618406    -5.308158     0.460659      26.99
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name = lig-etoh-frame_995
 C       2.646418     1.950393    -2.314970      75.95
 H       2.426201     2.687354    -3.049542      28.31
 C       3.456146     1.401214    -0.082974      66.62
 H       3.701247     1.925714     0.926263      23.50
 C       4.178854     0.337468    -0.530064      26.24
 O       4.964905    -0.510337     0.222202     272.08
 C       5.064294    -0.701174     1.613181     128.19
 H       4.039909    -0.648292     1.915308      28.13
 H       5.773901    -0.114114     2.099417      27.51
 H       5.290270    -1.634944     1.785415      29.19
 C       4.155154     0.152615    -1.898529      26.13
 O       4.659924    -1.097146    -2.352958     186.58
 H       4.931530    -1.428436    -1.404148      21.27
 C       3.514494     1.003927    -2.802325      65.40
 H       3.689785     1.017502    -3.926657      16.90
 C       2.638660     2.285253    -0.894544      68.10
 C       1.895073     3.473105    -0.377480      92.90
 H       1.978542     4.394632    -1.191924      18.76
 O       2.379160     3.581713     0.982171     339.16
 H       2.388922     4.468713     1.340792      30.02
 C       0.363224     3.323326    -0.353450      72.83
 H       0.025802     2.856143    -1.277279      23.34
 C      -0.322195     4.536002     0.361764      93.07
 O       0.177818     5.720172    -0.423209     155.27
 H      -0.018340     5.702051    -1.492922      25.17
 H       0.066626     4.721424     1.431229      23.80
 H      -1.470709     4.281035     0.433941      23.22
 C      -0.851246    -1.298907    -0.529396      49.79
 H      -0.259997    -2.299000    -0.748072      22.23
 C      -3.015251    -0.001221    -0.351383      56.97
 H      -3.900978     0.193597    -0.866467      22.29
 C      -2.166577     1.110685    -0.129664      -1.25
 O      -2.732792     2.487672     0.062118     140.81
 C      -4.187202     2.642098    -0.358326     127.90
 H      -4.948490     2.176901     0.119281      28.52
 H      -4.525288     3.668397    -0.095047      26.91
 H      -4.227970     2.450175    -1.317042      29.47
 C      -0.784023     1.068544     0.199569      -6.99
 O       0.116857     2.144128     0.565622      92.20
 C      -0.025511    -0.179977    -0.058070       4.14
 H       0.800336    -0.192601     0.608777      22.89
 C      -2.215582    -1.213217    -0.645523      13.83
 C      -3.048418    -2.493071    -1.188892      92.44
 H      -3.890031    -2.095677    -1.845735      25.30
 O      -2.168681    -3.152747    -2.135097     259.24
 H      -2.394445    -4.076478    -2.160496      22.81
 C      -3.557170    -3.351993    -0.054511     113.95
 H      -2.780304    -3.658720     0.587817      25.00
 O      -4.287783    -2.538171     0.722283     349.71
 H      -4.532530    -2.954482     1.458287      32.45
 C      -4.263403    -4.742340    -0.422261      83.78
 O      -3.373786    -5.573893    -1.352094     280.65
 H      -2.738537    -6.157683    -0.542844      22.35
 H      -5.169759    -4.271126    -1.018652      26.27
 H      -4.686811    -5.192196     0.451983      29.42
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name = lig-etoh-frame_996
 C       2.701836     1.996794    -2.267818      67.47
 H       2.325976     2.675596    -3.045122      22.43
 C       3.458635     1.497690    -0.003590      62.85
 H       3.547912     1.693993     1.116550      20.93
 C       4.175569     0.374169    -0.539717      26.24
 O       4.962595    -0.479105     0.162896     233.72
 C       5.055137    -0.727501     1.599590      89.62
 H       4.037224    -0.536507     2.124570      26.68
 H       5.753172     0.040589     2.147280      24.80
 H       5.376081    -1.957126     1.807597      23.03
 C       4.113692     0.073955    -1.931223      40.92
 O       4.672942    -1.046854    -2.384541     165.07
 H       5.364023    -1.329673    -1.567380      22.44
 C       3.484965     0.908813    -2.836156      78.83
 H       3.815973     0.990170    -3.903843      25.57
 C       2.660159     2.301713    -0.912872      57.21
 C       1.962876     3.485575    -0.423492     130.06
 H       2.167556     4.503941    -0.613710      21.96
 O       2.315998     3.582381     0.976628     315.63
 H       2.090437     4.507954     1.433507      26.67
 C       0.307245     3.213583    -0.275373      78.58
 H      -0.182268     3.027336    -1.281848      23.18
 C      -0.275900     4.510219     0.321721     103.38
 O       0.151413     5.794869    -0.394635     208.96
 H      -0.017796     5.722781    -1.273382      31.90
 H       0.233689     4.776019     1.222046      25.50
 H      -1.301367     4.453277     0.500112      26.93
 C      -0.799885    -1.242376    -0.555162      91.20
 H      -0.411709    -2.151903    -0.871989      26.39
 C      -2.915874    -0.040277    -0.327690      46.43
 H      -3.924877     0.063795    -0.859296      18.35
 C      -2.180325     1.181207    -0.107687       3.67
 O      -2.769819     2.450958     0.049535     168.16
 C      -4.124631     2.640557    -0.291876     105.39
 H      -5.187309     1.972679    -0.070361      21.31
 H      -4.432287     3.705599    -0.373600      24.22
 H      -4.573279     2.657647    -1.756210      21.18
 C      -0.754135     1.017236     0.159462       8.27
 O       0.131109     2.085211     0.585110     143.02
 C      -0.125201    -0.252007    -0.032744      53.94
 H       1.019453    -0.240056     0.254907      23.03
 C      -2.252470    -1.219169    -0.710238       5.94
 C      -2.992418    -2.474194    -1.142468      96.60
 H      -3.855958    -2.180635    -1.705732      26.23
 O      -2.162222    -3.177585    -2.158205     207.51
 H      -2.209165    -4.232335    -1.949539      18.29
 C      -3.519369    -3.455382    -0.007410      85.10
 H      -2.680738    -3.841902     0.742574      22.84
 O      -4.340760    -2.499333     0.690730     249.79
 H      -4.814092    -3.089488     1.447548      26.91
 C      -4.337286    -4.693474    -0.476313      90.66
 O      -3.372151    -5.532857    -1.336645     337.80
 H      -2.817752    -5.924285    -0.803146      34.04
 H      -5.353742    -4.775268    -0.953652      26.22
 H      -4.630089    -5.263117     0.481567      27.41
55
name = lig-etoh-frame_997
 C       2.777619     2.026128    -2.270308      51.01
 H       2.033638     2.600924    -2.857347      20.30
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 C       3.463573     1.568744     0.059766      35.42
 H       3.435311     1.605853     1.089641      21.05
 C       4.126185     0.457395    -0.527553      16.53
 O       4.991972    -0.482623     0.115561     219.36
 C       5.024142    -0.746994     1.611881     121.41
 H       4.165366    -0.536958     2.185931      30.10
 H       5.696991    -0.032909     1.975490      28.42
 H       5.368534    -1.713486     1.625206      28.25
 C       4.061225     0.012156    -1.956077      25.19
 O       4.743389    -1.038735    -2.411446     246.82
 H       5.469099    -1.298823    -2.005744      30.68
 C       3.435820     0.870190    -2.848919      87.44
 H       3.736983     0.775347    -3.873590      28.71
 C       2.725813     2.287184    -0.929701      55.09
 C       1.964332     3.514582    -0.396349     108.86
 H       2.347810     4.580889    -0.666610      21.72
 O       2.269312     3.583766     1.016584     338.78
 H       1.873649     4.405665     1.292542      27.74
 C       0.277923     3.138742    -0.252066      81.36
 H      -0.289662     3.209112    -1.196007      22.93
 C      -0.203627     4.525927     0.284868      88.17
 O       0.108642     5.847016    -0.352402     161.78
 H      -0.025547     5.663237    -1.432937      25.37
 H       0.311450     4.649433     1.278394      23.91
 H      -1.347880     4.646493     0.496688      23.53
 C      -0.836998    -1.276927    -0.606537       5.24
 H      -0.331327    -2.226522    -0.955804      25.58
 C      -2.827902    -0.043865    -0.372922      56.40
 H      -3.937533    -0.070904    -0.460139      23.45
 C      -2.168113     1.218260    -0.058166      21.76
 O      -2.819291     2.403268     0.031506     184.94
 C      -4.152999     2.651874    -0.313178     112.87
 H      -4.691890     1.904686     0.054918      26.35
 H      -4.157184     3.760926    -0.264574      23.94
 H      -4.328507     2.565700    -1.677699      22.80
 C      -0.732563     1.002400     0.119106      -8.13
 O       0.119337     2.008084     0.607469     174.98
 C      -0.154103    -0.227274     0.030612      72.17
 H       0.861417    -0.351814    -0.262823      24.30
 C      -2.249070    -1.225445    -0.745344      35.22
 C      -2.923195    -2.485321    -1.132835      90.40
 H      -3.983180    -2.220365    -1.525062      24.88
 O      -2.148718    -3.212054    -2.168420     235.63
 H      -2.162426    -4.082289    -1.798657      22.05
 C      -3.482440    -3.524646     0.039600      75.46
 H      -2.677013    -3.960206     0.599093      24.09
 O      -4.415899    -2.477690     0.683295     208.84
 H      -5.034185    -2.954097     1.433699      27.20
 C      -4.383049    -4.696363    -0.517134     101.33
 O      -3.408661    -5.471065    -1.320978     296.34
 H      -2.661222    -6.009768    -0.655914      24.53
 H      -5.322066    -4.862185    -1.070330      25.80
 H      -4.380359    -5.324658     0.363502      27.39
55
name = lig-etoh-frame_998
 C       2.819106     2.028602    -2.319368      54.71
 H       1.945218     2.505308    -2.755076      19.41
 C       3.488391     1.574784     0.051513      34.76
 H       3.357810     1.757607     1.263072      17.85
 C       4.094007     0.483796    -0.519432      20.90
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 O       5.007979    -0.486892     0.090516     190.69
 C       5.002838    -0.709684     1.575584      94.46
 H       3.975609    -0.631826     2.143256      25.99
 H       5.889259    -0.048818     1.945434      25.12
 H       5.439039    -1.874774     1.595145      23.94
 C       4.016412     0.021279    -1.916968      19.49
 O       4.807812    -1.063287    -2.476700     153.80
 H       5.818286    -1.274501    -2.078218      26.32
 C       3.386784     0.868395    -2.842600      84.68
 H       3.392382     0.517953    -3.974006      24.23
 C       2.795808     2.316549    -0.897458      58.77
 C       1.941274     3.514932    -0.337423     110.11
 H       2.175111     4.283046    -1.116926      25.27
 O       2.238503     3.582729     1.072157     342.74
 H       1.804779     4.388615     1.309830      28.51
 C       0.290905     3.170111    -0.288728      60.49
 H      -0.259771     2.927610    -1.224977      23.42
 C      -0.173237     4.579736     0.323769     108.07
 O       0.062759     5.855440    -0.348777     233.68
 H       0.137949     5.748700    -1.339787      29.02
 H       0.155450     4.536648     1.369728      24.60
 H      -1.222664     4.576039     0.437527      25.25
 C      -0.891207    -1.352766    -0.646273      15.41
 H      -0.206575    -2.176047    -0.908482      24.18
 C      -2.806504     0.006932    -0.425504      58.71
 H      -3.861420    -0.069243    -0.078227      24.63
 C      -2.143797     1.164447    -0.023798      26.33
 O      -2.816354     2.371157     0.031211     185.11
 C      -4.164227     2.683844    -0.388847     107.39
 H      -4.699881     1.843027     0.401234      22.44
 H      -4.251297     3.690093     0.050372      24.55
 H      -3.956217     2.256680    -1.460573      23.15
 C      -0.753231     1.046368     0.109948      -3.62
 O       0.103133     1.958023     0.619058     136.86
 C      -0.148151    -0.239276     0.025130      25.66
 H       0.892102    -0.264584    -0.451774      22.73
 C      -2.186537    -1.254890    -0.754033      40.70
 C      -2.922369    -2.536253    -1.143305     107.63
 H      -3.863542    -2.262306    -1.498679      27.21
 O      -2.137735    -3.223305    -2.159765     230.14
 H      -2.173092    -4.157762    -1.820622      19.93
 C      -3.515880    -3.498155     0.042807      74.43
 H      -2.674446    -4.018389     0.679455      23.01
 O      -4.480915    -2.486957     0.686919     283.00
 H      -4.965905    -2.779114     1.346857      33.53
 C      -4.347284    -4.749946    -0.518872      82.58
 O      -3.415742    -5.432599    -1.310808     307.99
 H      -2.908391    -6.041065    -0.605139      25.08
 H      -5.291093    -4.457556    -1.186564      25.27
 H      -4.515512    -5.395809     0.383368      27.00
55
name = lig-etoh-frame_999
 C       2.798862     2.034168    -2.322007      68.01
 H       2.025734     2.529459    -2.964087      20.31
 C       3.507347     1.561127     0.053957      19.21
 H       3.508468     1.884154     0.971905      23.27
 C       4.130387     0.396978    -0.524689      25.50
 O       4.997996    -0.475873     0.088776     240.38
 C       5.021590    -0.688217     1.511139     120.73
 H       4.049896    -0.659570     1.876562      29.78
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 H       5.754268    -0.117231     2.049533      27.54
 H       5.273479    -1.734053     1.691862      27.11
 C       4.024400     0.052951    -1.876307      32.61
 O       4.864546    -1.086970    -2.538503     171.95
 H       5.729287    -0.970445    -1.984557      28.36
 C       3.343318     0.844683    -2.846604      40.32
 H       3.076291     0.572048    -3.765172      24.49
 C       2.843572     2.376512    -0.869620      75.45
 C       1.898443     3.426719    -0.315351     107.37
 H       1.879834     4.141013    -1.188464      26.98
 O       2.223645     3.607044     1.106553     307.05
 H       1.865413     4.497545     1.556795      24.92
 C       0.349523     3.251162    -0.338144      44.45
 H      -0.035099     2.700532    -1.230695      22.00
 C      -0.208781     4.604539     0.374742     101.64
 O       0.037140     5.844136    -0.347286     229.39
 H       0.255841     5.735470    -1.287497      30.29
 H       0.084698     4.667290     1.440655      23.62
 H      -1.350378     4.373274     0.403355      22.76
 C      -0.805947    -1.380844    -0.620365      57.57
 H      -0.255963    -2.260711    -0.866270      26.36
 C      -2.834648     0.013335    -0.466899      51.65
 H      -3.828221    -0.029265     0.086513      24.42
 C      -2.150911     1.110130    -0.025908      21.96
 O      -2.745958     2.367315     0.068759     140.00
 C      -4.149274     2.626403    -0.370988      89.82
 H      -4.946366     2.221921     0.171859      26.31
 H      -4.532420     3.650178     0.023114      23.91
 H      -4.143614     2.151258    -1.749307      21.76
 C      -0.755943     1.040022     0.130300      -2.66
 O       0.100795     1.980330     0.623004      89.62
 C      -0.146319    -0.278733    -0.091370      39.78
 H       0.929867    -0.082082    -0.129255      23.93
 C      -2.208589    -1.292832    -0.750507      -8.61
 C      -2.965374    -2.592597    -1.145846      98.48
 H      -3.890232    -2.214561    -1.787656      23.54
 O      -2.126337    -3.232610    -2.132288     210.14
 H      -2.228649    -4.288911    -2.076584      17.42
 C      -3.584315    -3.439910     0.044949     100.64
 H      -2.873158    -3.741133     0.822383      24.68
 O      -4.505119    -2.505779     0.662138     238.43
 H      -4.925962    -2.892179     1.623116      26.70
 C      -4.306023    -4.752998    -0.485227      98.50
 O      -3.401572    -5.440071    -1.309610     330.50
 H      -3.038490    -6.095855    -0.720699      28.37
 H      -5.021882    -4.212385    -1.032222      28.20
 H      -4.956785    -5.317174     0.259892      28.26
55
name = lig-etoh-frame_1000
 C       2.732403     2.041730    -2.280131      76.82
 H       2.271025     2.608770    -3.071630      25.61
 C       3.539455     1.516818    -0.006308     115.68
 H       3.789011     1.984467     1.125952      23.40
 C       4.179746     0.309324    -0.521652      51.48
 O       5.011267    -0.477346     0.099009     232.19
 C       5.031114    -0.676928     1.451014     102.43
 H       3.914690    -0.493208     1.801035      26.21
 H       5.608162     0.039368     2.127217      25.34
 H       5.265050    -1.836771     1.675054      24.24
 C       4.070586     0.048664    -1.924249      38.51
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O	4.892817	-1.061446	-2.557186	203.24
H	5.586140	-0.904495	-1.983118	30.15
C	3.298728	0.843602	-2.777019	58.89
H	2.934052	0.614180	-3.878643	19.59
C	2.859196	2.407124	-0.886651	80.04
C	1.844167	3.344844	-0.314177	110.55
H	1.894732	4.377015	-0.849486	21.09
O	2.225830	3.653134	1.125521	363.46
H	2.071921	4.488076	1.576972	29.10
C	0.429500	3.286675	-0.334466	56.90
H	0.117791	2.985314	-1.342621	23.48
C	-0.311524	4.584095	0.383621	94.57
O	0.013372	5.825663	-0.333294	176.37
H	0.360714	5.573559	-1.354220	24.57
H	0.096919	4.843453	1.384833	23.47
H	-1.350080	4.298618	0.372742	24.35
C	-0.720446	-1.402215	-0.581031	30.73
H	-0.337859	-2.454283	-0.820085	22.31
C	-2.897354	-0.072901	-0.480799	55.80
H	-3.928876	-0.045824	-0.197681	26.10
C	-2.146131	1.101091	-0.052419	4.54
O	-2.696674	2.384371	0.122263	147.71
C	-4.117034	2.552288	-0.388631	119.23
H	-5.176471	2.013106	0.013391	23.92
H	-4.334933	3.625405	-0.439541	26.82
H	-4.544192	2.499686	-1.276237	27.69
C	-0.738764	0.967039	0.154571	21.36
O	0.096455	2.046556	0.624601	53.39
C	-0.114218	-0.240054	-0.220691	50.53
H	0.918954	-0.188900	0.267636	24.84
C	-2.253836	-1.316128	-0.729720	-33.83
C	-3.047677	-2.608542	-1.173791	92.96
H	-3.785858	-2.287157	-1.827822	25.03
O	-2.103491	-3.264189	-2.102622	244.66
H	-2.386251	-4.136056	-2.221630	23.36
C	-3.642578	-3.388189	0.075439	101.38
H	-2.856959	-3.465546	0.907535	23.53
O	-4.552101	-2.530641	0.655210	286.94
H	-4.516883	-2.926982	1.602086	27.58
C	-4.292823	-4.684936	-0.429988	82.66
O	-3.387295	-5.474135	-1.309813	220.94
H	-2.940851	-6.437107	-0.787212	21.81
H	-4.990180	-4.093400	-1.256804	24.32
H	-5.083717	-5.227973	0.077032	26.97